The Fourteenth International Symposium on Artificial Life and Robotics 2009 (AROB 14th '09),
B-Con Plaza, Beppu, Oita, Japan, February 5 - 7, 2009

Energy Levels by a Simple Shooting Scheme for a Periodic Orbit

Kazuhiro Kubo, Tokuzo Shimada
Department of Physics, Meiji University
Higashi-Mita 1-1, Kawasaki, Kanagawa 214, Japan

We revisit the periodic orbit theory for anisotropic Kepler problem, which is an important playground for the quantum chaos. In order to explore the periodic orbit Gutzwiller devised an iteration scheme, which computes Fourier coefficients of the orbit iteratively. Here we note in a nutshell all one needs is the primary periodic orbit. We propose an alternative scheme taking account for the symmetry of the target trajectory and the scaling property of the AKP equation of motion. We show a simple shooting scheme gives almost immediately the final periodic orbit.

Key words: quantum chaos, anisotropic Kepler problem, shooting method, periodic orbit theory

I. INTRODUCTION

Recently by the advent of nano-scale devices the handling of various quantum systems in a laboratory becomes viable. A good example is a quantum dot, which confines electrons in a two dimensional region of several hundreds nano-meters in size. This device, under an external magnetic field and at low temperatures, exhibits electric conductance depending on the shape of the region of confinement; it depends whether the region allows regular classical orbit or the region induces the chaotic orbit. Then, natural question arises; if the classical theory for a system involves chaos, does it somehow affect the quantum behavior of the system? The solution of this question will give a clue for the real foundation of quantum theory.

Two possible approaches to this problem may be envisaged; random matrix theory (RMT) and periodic orbit theory (POT). In RMT, the Hamiltonian of the system is approximated by a matrix whose elements are random numbers. The symmetry of the system dictates the type of the ensemble of the random matrices. For instance, for large nuclei, the nearest neighbor spacing distribution of the energy level agrees well with that of a real symmetric random matrix (rather than a simple Poisson distribution). Then, in POT, based on the Feynman's path integral, the quantum characteristics in the semi-classical regime is estimated from classical orbits. Therefore, it is suited to investigate the classical-quantum correspondence. For instance, it is a vital tool for the analysis of the shell effect in the total energy of nuclei.

In a series of works [2–4], Gutzwiller studied various spherically symmetric potentials. These are all integrable cases because the separation of variables is possible; the classical orbits are regular. These may be regarded as a preparation for the next step towards the POT. In a seminal work [5], Gutzwiller extended the work to a non-integrable Hamiltonian system, whose classical trajectory is chaotic. Gutzwiller's quantization condition is

$$S(E) = 2\pi\hbar(n + \ell(E)/4). \tag{1}$$

Here, E is the total energy of the chosen periodic orbit and S is the action integral

$$S(E) = \oint p_i dq_i, \tag{2}$$

along the periodic orbit for one period, and ℓ is a number of conjugate points along the periodic orbit. The energy levels E_n are given by solving the condition (1). The condition (1) is then applied to anisotropic Kepler problem (AKP) and the resulting energy levels are in good agreement with those by solving the Schrödinger equation.

As is well known, the energy levels of an ordinary Kepler problem are given by $-1/n^2$ in appropriate units with the principal quantum number n. In AKP, the energy levels turn out again to be proportional to $-1/n^2$, and the anisotropy affects the proportionality coefficient γ^2. ($\gamma = 1$ for the Kepler problem). In order to compute the value of γ for a certain anisotropy, it is necessary to find a periodic orbit as a solution of the equation of motion of AKP. In [5], a fundamental periodic orbit and its γ are calculated using an iteration scheme. However, this iteration scheme is somewhat elaborated and requires large computation time.

In this paper, we present an alternative scheme to find the fundamental periodic orbit by a simple shooting scheme. In our method a scaling property of the system is fully accounted and the symmetry of the orbit shape helps to reduce the shooting analysis to only one-dimensional. The resulting γ is in good agreement with the Gutzwiller's value.

II. ANISOTROPIC KEPLER PROBLEM

The AKP is a Kepler problem with an anisotropic mass tensor. It includes the motion of an electron confine in a semiconductor. The Hamiltonian of the two-dimensional AKP is

$$H(p,\ q) = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} - \frac{e^2}{\kappa\sqrt{q_1^2 + q_2^2}}. \tag{3}$$

with $(q_1,\ q_2)$ the position of the electron and $(p_1,\ p_2)$ the conjugate momentum. The m_1, m_2 are the diagonal elements of the electronic mass tensor and we choose $m_1 > m_2$ (q_1 is 'the heavy axis').

The dimensionless variables for energy, length, frequency are respectively defined in the units

$$E_0 = \frac{m_0 e^4}{2\kappa^2\hbar^2},\ a_0 = \frac{\kappa\hbar^2}{m_0 e^2},\ \omega_0 = \frac{m_0 e^4}{\kappa^2\hbar^3} \tag{4}$$

with $m_0 = \sqrt{m_1 m_2}$. Dimensionless coordinates and temporal parameter are respectively defined by

$$\xi \equiv \frac{q_1}{\sqrt{\mu} a_0},\ \eta \equiv \frac{q_2}{\sqrt{\nu} a_0},\ \tau \equiv \omega_0 t. \tag{5}$$

In order to write the Hamiltonian (and action) with the dimensionless variables, it is convenient to pass through the Lagrangian formalism. The Lagrangian in terms of the dimensionless variables is obtained as

$$\mathcal{L} \equiv \frac{L}{E_0} = \xi'^2 + \eta'^2 + \frac{2}{\sqrt{\mu\xi^2 + \nu\eta^2}} \tag{6}$$

where the prime indicates the derivative with respect to τ and the relation $d/dt = \omega_0 d/d\tau$ is used. The dimensionless conjugate momentum is

$$p_\xi = \frac{\partial \mathcal{L}}{\partial \xi'} = 2\xi', \quad p_\eta = \frac{\partial \mathcal{L}}{\partial \eta'} = 2\eta', \tag{7}$$

and therefore the dimensionless Hamiltonian is given by

$$h \equiv \frac{H}{E_0} = \frac{p_\xi^2}{4} + \frac{p_\eta^2}{4} - \frac{2}{\sqrt{\mu\xi^2 + \nu\eta^2}}, \tag{8}$$

with $\mu = 1/\nu = \sqrt{m_2/m_1} < 1$. The Hamilton equation in the dimensionless variables is

$$\begin{aligned} \xi' &= \frac{\partial h}{\partial p_\xi} = \frac{p_\xi}{2}, \quad p'_\xi = -\frac{\partial h}{\partial \xi} = -\frac{2\mu\xi}{(\mu\xi^2 + \nu\eta^2)^{3/2}}, \\ \eta' &= \frac{\partial h}{\partial p_\eta} = \frac{p_\eta}{2}, \quad p'_\eta = -\frac{\partial h}{\partial \eta} = -\frac{2\nu\eta}{(\mu\xi^2 + \nu\eta^2)^{3/2}}. \end{aligned} \tag{9}$$

The energy conservation equation calculated from Eq. (8) with Eq. (7) is

$$\xi'^2 + \eta'^2 - \frac{2}{\sqrt{\mu\xi^2 + \nu\eta^2}} = \epsilon. \tag{10}$$

Only the bound states are discussed below, hence $\epsilon < 0$ and trajectories in the $\xi\eta$ plane are all limited inside an ellipse

$$\mu\xi^2 + \nu\eta^2 = \left(\frac{2}{\epsilon}\right)^2. \tag{11}$$

The form of the energy in (10) is quadratic in ξ' and η' and it is homogeneous in ξ and η. Therefore we can use the virial theorem to write the action from Eq. (2) as

$$\frac{S}{\hbar} = \int (\xi'^2 + \eta'^2) d\tau = -\epsilon \frac{2\pi}{\omega}. \tag{12}$$

Here, ω is the dimensionless angular frequency in the unit ω_0.

In the case of ordinary Kepler problem, the shapes of trajectories in bound states are all elliptic except the radial motion. In the units (4), the total energy for the elliptic orbit is represented by

$$\epsilon = -\bar{\alpha}^2 \bar{\omega}^2. \tag{13}$$

Dimensionless variables $\bar{\alpha}$ and $\bar{\omega}$ ()correspond to the major radius and angular frequency of the elliptic orbit respectively. Similarly, the Kepler's third law is given by

$$\bar{\alpha}^3 \bar{\omega}^2 = 1. \tag{14}$$

These relations (13), (14) can be extended to the case of AKP. The energy is

$$\epsilon = -\alpha^2 \omega^2. \tag{15}$$

Again these are the dimensionless energy, size, frequency of the AKP in the units (4).

The counterpart of Eq. (14) is introduced by

$$\gamma \equiv \alpha^3 \omega^2. \tag{16}$$

For each periodic orbit, γ takes a different value which depends only on $m = (\mu - \nu)/(\mu + \nu)$, the degree of the anisotropy. It should be noted that for a non-anisotropic case, i.e. $m = 0$, a relation $\gamma(0) = 1$ is satisfied, which is the Kepler's third law.

By the change of variables from $(\alpha,\ \omega)$ to $(\epsilon,\ \gamma)$, the action in Eq. (12) is rewritten as

$$S = 2\pi\hbar \frac{\gamma(m)}{\sqrt{|\epsilon|}}. \tag{17}$$

By the help of the quantization condition (1), the energy levels of the AKP turn out to be

$$\epsilon_n = -\frac{\gamma^2}{n + \frac{\ell}{4}^2}. \tag{18}$$

According to Eq. (18), if the value of γ and the number of conjugate points are known for the particular periodic orbit, then the energy levels of the AKP can be estimated when the degree of anisotropy m is fixed.

For the fundamental periodic orbit discussed below, ℓ equals to 2 and 4 for the two and three dimensional cases respectively [5].

III. GUTZWILLER'S ITERATION SCHEME

In order to compute the value of γ, the search of the periodic orbit is needed. The target is the primary periodic orbit. Its shape is oval; mirror symmetric about both ξ, η axes. For $m = 0$ (the ordinary Kepler problem), the shape is simply a circle, while with anisotropy, one cannot derive the exact solution analytically. To search this orbit, an iteration scheme is devised in [5]. In this scheme complex coordinates are expanded in Fourier series as

$$\xi + i\eta = \alpha \sum_{-\infty}^{\infty} \alpha_j z^{2j+1},$$

$$\xi - i\eta = \alpha \sum_{-\infty}^{\infty} \beta_j z^{2j+1},\ \beta_j = \alpha_{-j-1} \in \mathcal{R}$$

with $z = \exp(i\omega\tau)$. Because the coefficients are calculated by a fixed algorithm below, the scale factor α is needed. The iteration starts from an initial configuration $\alpha_0 = 1, \alpha_1 = \alpha_2 = \cdots = 0$ corresponding to a circle, which is a primary orbit for a Kepler problem without anisotropy. At each step of the iteration procedure, the higher mode Fourie coefficients are computed from the lower by a couple of recurrence relations (derived from the equation of motion and the energy conservation). As the iteration proceeds, the set of Fourie coefficients is thus improved towards the final solution and the circle at the initial time is deformed to the primary orbit of AKP. At the end of the iteration the value of γ is calculated from the Fourie coefficients.

This scheme is advantageous in that the orbit is always closed and the symmetry is respected in every step. However, the number of Fourier coefficients grows exponentially. Therefore it is necessary to truncate the small higher frequency terms. In order to improve both the accuracy huge memory space and long computation time are then required. The decision of whether sufficient convergence is reached or not is difficult, because the convergence is slow and oscillatory as we will reproduce below [7].

IV. PERIODIC ORBIT SEARCH BY A SIMPLE SHOOTING SCHEME

Now let us propose an alternative scheme which uses a shooting method integrating (9). The symmetry of the target orbit simplifies the search; a one-dimensional search is sufficient.

From Eqs. (15), (16) we obtain

$$\gamma = \frac{|\epsilon|^{\frac{3}{2}}}{\omega}, \quad \alpha = \frac{\sqrt{|\epsilon|}}{\omega}. \tag{19}$$

Therefore, γ and α can be worked out by measuring the period ($T = 2\pi/\omega$) of the final orbit with energy ϵ. (The energy can be chosen at an arbitrary value under the scaling). All we need is the precise determination of the period, that is, the precise determination of initial conditions in the shooting scheme. Therefore, this scheme is free from the problems of convergence and huge memory.

A. Choice of energy and the families of trajectories

Let us consider the scaling property of the AKP equation of motion. It is form invariant under the transformation

$$\begin{aligned} \xi(\tau) &\to \tilde{\xi}(\tilde{\tau}) = s \cdot \xi(\tau), \\ \eta(\tau) &\to \tilde{\eta}(\tilde{\tau}) = s \cdot \eta(\tau), \\ \epsilon &\to \tilde{\epsilon} \ = s^{-1} \cdot \epsilon \\ \tau &\to \tilde{\tau} = s^{\frac{3}{2}} \cdot \tau. \end{aligned} \tag{20}$$

Accordingly the period is scaled as $T \to s^{3/2} \cdot T$. For the scale of the orbit, $\alpha \to s \cdot \alpha$ just like ξ and η.

This scaling property implies that there is a one-parameter (s) family of orbits. What we need is to determine the family to which the primary periodic orbit belongs as a member. Therefore we can pick an arbitrary ϵ for the shooting. Another choice of ϵ will search out another orbit but in the same family. Since the combination $\gamma \equiv \alpha^3\omega^2$ is scale invariant, any member in the same family will give the same γ.

B. The shooting scheme

Let us show that the search for the primary orbit (with reflection symmetry with respect to both ξ and η axes) requires only a one dimensional shooting scheme. From the symmetry, it definitely passes through the ξ axis. So we can choose the initial point on the ξ axis $(\xi_0, 0)$. That is, we choose the ξ axis as a Poincaré surface of section. From the symmetry it suffices to take $\xi_0 > 0$. Also from the symmetry the initial momentum must be then at right angles to the ξ axis; p_ξ must be vanishing ($(p_\xi)_0 = 0$). Furthermore, p_η is computed from ξ_0 via the energy conservation (10). Thus, the initial condition is given by

$$(\xi,\ \eta,\ p_\xi,\ p_\eta) = (\xi_0,\ 0,\ 0,\ p_\eta(\xi_0)). \tag{21}$$

with $p_\eta = 2\sqrt{\frac{2}{\sqrt{\mu}\xi_0} + \epsilon}$. Therefore one-dimensional search, varying ξ_0 as a parameter, is sufficient. The bound for ξ_0 is $0 < \xi_0 < \xi_{max} \equiv 2/\sqrt{\mu}|\epsilon|$.

From this initial point the Hamilton equation is integrated until the trajectory crosses again the Poincaré surface of section ($\eta = 0$). We call this first intersection (after the initial point) as the final point.

The constraint in the shooting scheme is two-fold

$$\xi_1 = \xi_0, \quad (p_\xi)_1 = 0. \tag{22}$$

The integration preserves the energy so that the condition $(p_\eta)_1 = (p_\eta)_0$ automatically follows from $\xi_1 = \xi_0$. The integration is iteratively repeated until the differences $\delta\xi \equiv \xi_1 - \xi_0$ and $(p_\xi)_1$ reach zero.

The constraint (22) is put on the first crossing of the Poincaré section so that it is strong enough to single out the primary orbit. In fact there is (at least) one other solution which is symmetric with respect to both ξ and η axes, but it is oscillatory and after many crossings it comes back to the starting point.

C. The initial value ξ_0^* of the primary orbit and theγ in the shooting scheme

To be explicit let us choose the anisotropy $m = 0.899$ ($\mu = 0.231$) (the germanium) and pick $\epsilon = -0.1$. Fig. 1 is a plot of $\delta\xi$ and $(p_\xi)_1$ as functions of ξ_0. We observe $\delta\xi$ changes the sign as ξ_0 passes a critical value of $\xi_0^* \approx 4.9$. This ξ_0^* is the initial value of the primary periodic orbit. Using the bi-section method for ξ_0^*, we obtain more precise value $\xi_0^* = 4.893087$. The period of

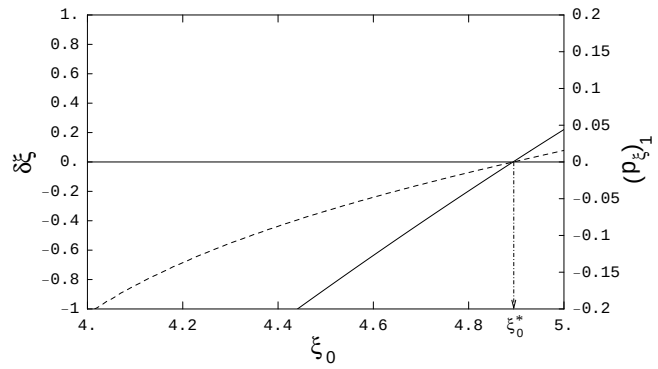

FIG. 1: ξ(solid line), $(p_\xi)_1$(dashed line) versus ξ_0. $\epsilon =$ 0.1.

this solution turns out $T = 151.2541$ and the angular frequency is $\omega = 4.154059 \times 10^{-2}$.

With this ω and $\epsilon = -0.1$ we obtain from (19)

$$\gamma = 0.7612500, \quad \alpha = 7.612500. \tag{23}$$

V. COMPARISON BETWEEN THE TWO SCHEMES

Let us reproduce the computation in [5]. The fundamental periodic orbit and γ may be computed at every iteration step, and hence we can compare them with those by our scheme.

1) *The comparison of orbits.* In Fig. 2, the orbits at several steps of the iteration scheme are compared with the orbit obtained by our shooting scheme. The latter is normalized by the scale factor α in Eq. (23). The zeroth step orbit is a unit circle; as the iteration proceeds, it approaches oscillatory the orbit obtained by the shooting scheme.

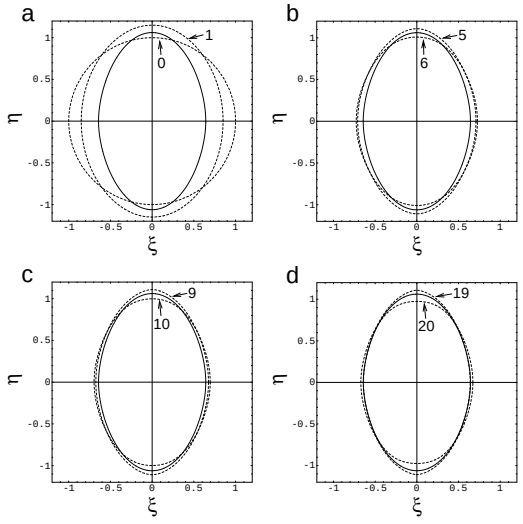

FIG. 2: The orbits from the iteration scheme (dashed lines) as compared with the one from the shooting scheme (the solid line). Numbers indicate the iteration steps.

2) *Comparison of the parameter γ.* As seen in Fig. 3, γ in the iteration scheme decreases in oscillation, but after the 17th step, the decrease becomes slower and the oscillation remains. Therefore it is difficult to judge the convergence. The asymptote may be slightly above γ determined by the shooting scheme, but it may also be in agreement if iteration is continued further. But the necessary number of the Fourier coefficients is approximately 2^{n+1} in the n-th iteration step and such calculation is practically difficult.

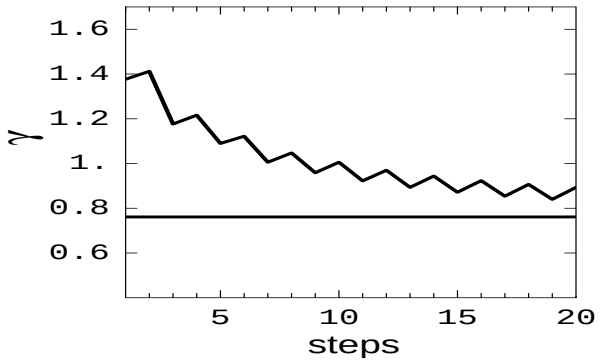

FIG. 3: Comparison of iteration result with that by shooting (23)(horizontal line) up to 20th step. $m = 0.899$ (Ge case).

In Summary, in Gutzwiller's scheme one has to compute exponentially increasing number of Fourier coefficients at each step of the iteration, while in our shooting scheme, it is just sufficient to integrate the orbit from the initial point to the first Poincaré section at each step of the iteration.

[1] R. P. Feynman, Rev. Mod. Phys. **20**, 367 (1948).
[2] M. C. Gutzwiller, J. Math. Phys. **8**, 1979 (1967).
[3] M. C. Gutzwiller, J. Math. Phys. **10**, 1004 (1969).
[4] M. C. Gutzwiller, J. Math. Phys. **11**, 1791 (1970).
[5] M. C. Gutzwiller, J. Math. Phys. **12**, 343 (1971).
[6] R. A. Faulkner, Phys. Rev. **184**, 713 (1969).
[7] This is remedied by a prescription [5]; make the variation small at chosen intervals.