STUDIA UBB PHYSICA, Vol. 60 (LX), 1, 2015, pp. 91-101
(RECOMMENDED CITATION)

Dedicated to Academician Professor Dr. Emil Burzo on His 80th Anniversary

COLLECTIVE BEHAVIOR OF COUPLED QUANTUM MECHANICAL OSCILLATORS

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ABSTRACT. A simple model of coupled oscillators is investigated from the perspective of quantum mechanics. The classical model of two oscillators connected by a common platform can be easily solved analytically, but the quantum system requires a numerical approach. We assume that both the oscillators and the platform are quantum objects in their respective ground states at start and they evolve in time as a connected system. By following numerically this time-evolution we investigate the dynamics of the oscillators and calculate an order parameter that characterizes their correlated time-evolution. We study the order parameter as a function of the oscillators initial state and compare the findings with the equivalent classical system. Interestingly, for a given parameter region we found an enhanced collective behavior in the quantum mechanical system.

Keywords*: nonlinear dynamics, collective behavior, quantum synchronization, coupled oscillators*

INTRODUCTION

Systems of coupled oscillators have provided great demonstrations of complex behaviour emerging from the interaction of simple system. Classical coupled oscillators have been thoroughly studied from the earliest observations of spontaneous synchronization by Huygens [1], and still are of great interest to physicists. Recent experimental studies conducted using metronomes on a moving platform [2] or a freely rotating platform [3], as well as detailed numerical

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studies of systems of pendulus [4], show that the possibility of spontaneous in-phase and anti-phase synchronization is an inherent property of such type of systems. On the other hand, it is easy to demonstrate that emergent synchronization only occurs in systems with driving and damping present, and depends on the system's parameters [5]. The simplest system of two oscillators attached to a common platform without driving or friction is exactly solvable and its degree of synchrony depends only on the initial positions of both oscillators.

If we take a closer look at this simplest system of coupled oscillators within the formalism of quantum mechanics, many of the classical properties of the oscillator systems translate into similar properties in the analogous quantum mechanical system. For instance, Y. F. Chen [6] demonstrated that the stationary coherent states of certain coupled oscillator systems possess the same shape as the classical trajectories of the system. If this holds true for the system we've selected here, we should observe similar dynamics in the quantum system and the classical one. Spontaneous synchronization should not be observed without energy dissipation or driving and the correlation between oscillators should follow a similar pattern with the classical case, being highly dependent on initial conditions. The system of coupled oscillators with dissipation has been studied by G. L. Giorgi et. al. [7] and indeed they have observed synchronization occurring between the oscillators average coordinates in a case they are connected to a common heat bath. This collective behavior depends mostly on the relevant physical parameters of the system, rather than the initial conditions. The case with driving has also been studied by Zhirov and Shepelyansky [8], and they established conditions for emergent synchronization in such systems.

Our aim here is quite modest, we intend to numerically study the collective behavior in a system of coupled quantum oscillators, using Pearson correlation between the expectation values of the oscillator coordinates as order parameter. As a quantum counterpart of the system considered by McDermott and Redmount [9], we assume that the oscillators and the platform they are attached to are initially independent quantum oscillators. They are initialized using their ground state wave functions shifted to match the desired starting positions. We intend to compare the numerical findings with the exact results obtained in the equivalent classical system.

CLASSICAL SYSTEM OF COUPLED OSCILLATORS

We consider a system of two oscillators with masses m coupled by springs of spring constants *k* to a common platform with mass *M* (Fig. 1). We denote by x_1 and x_2 the spring deformation values and by x_3 the absolute coordinate of the platform. We assume the ideal case where friction and driving are absent.

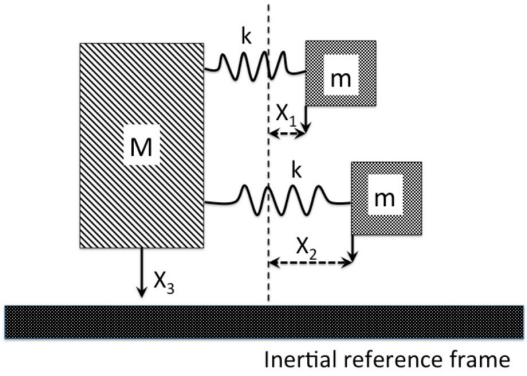

Fig. 1. The coupled oscillator system considered in our study.

The Lagrange function for this system is

$$L = \frac{1}{2}M\dot{x}_3^2 + \frac{1}{2}m(\dot{x}_1 + \dot{x}_3)^2 + \frac{1}{2}m(\dot{x}_2 + \dot{x}_3)^2 - \frac{1}{2}kx_1^2 - \frac{1}{2}kx_2^2, \qquad (1)$$

where the first term is the kinetic energy of the platform, the second and third terms stands for the kinetic energy of the oscillators relative to the chosen inertial reference frame, and the last two terms are the potential energies of the oscillators. The Euler-Lagrange equations of motion are:

$$\begin{aligned} M\ddot{x}_3 &= k(x_1 + x_2) \\ m\ddot{x}_1 &= -kx_1 - m\ddot{x}_3 \\ m\ddot{x}_2 &= -kx_2 - m\ddot{x}_3 \end{aligned} \qquad (2)$$

Eliminating the $\ddot{x}_3$ terms, we can derive a system of coupled differential equations yielding the dynamical evolution of the two masses m :

$$\begin{aligned} kx_1 + m\left(\frac{m+M}{2m+M}\right)\ddot{x}_1 - \frac{m^2}{2m+M}\ddot{x}_2 &= 0 \\ kx_2 + m\left(\frac{m+M}{2m+M}\right)\ddot{x}_2 - \frac{m^2}{2m+M}\ddot{x}_1 &= 0 \end{aligned} \qquad (3)$$

This system allows for an exact analytical solution. Assuming the initial positions of the oscillators $x_1(0) = 1, x_2(0) = a$ and that they are in rest relative to the platform $\dot{x}_1(0) = 0, \dot{x}_2(0) = 0$ the exact solutions for $x_1(t)$ and $x_2(t)$ are:

$$x_1(t) = \frac{1}{2}\left((1-a)\cos\frac{\sqrt{k}t}{\sqrt{m}} + (1+a)\cos\frac{k(2m+M)t}{\sqrt{kmM(2m+M)}} \right)$$
$$x_2(t) = \frac{1}{2}\left((a-1)\cos\frac{\sqrt{k}t}{\sqrt{m}} + (1+a)\cos\frac{k(2m+M)t}{\sqrt{kmM(2m+M)}} \right) \quad (4)$$

The Pearson correlation coefficient will be used as a measure of the synchronization level for the two oscillators. This coefficient will not distinguish between strong (phase-locked) and weak forms of synchronization. It will be denoted by *r* and it takes values between [−1,1]. For a completely in-phase synchronized state $r = 1$ and for a completely anti-phase synchronized state $r = -1$:

$$r = \frac{\langle x_1 x_2 \rangle_t - \langle x_1 \rangle_t \langle x_2 \rangle_t}{\sqrt{\langle x_1^2 \rangle_t - \langle x_1 \rangle_t^2}\sqrt{\langle x_2^2 \rangle_t - \langle x_2 \rangle_t^2}} \quad (5)$$

Here we denoted by $\langle x \rangle_t$ the time-average of quantity x. Taking into account that $\langle \cos(\alpha t) \rangle_t = 0$ and $\langle \cos(\alpha t)\cos(\beta t) \rangle_t = 0$ for all $\alpha \neq 0, \beta \neq 0$ by simple algebra one gets a result independent of m, k and M:

$$r = \frac{2a}{a^2 + 1} \quad (6)$$

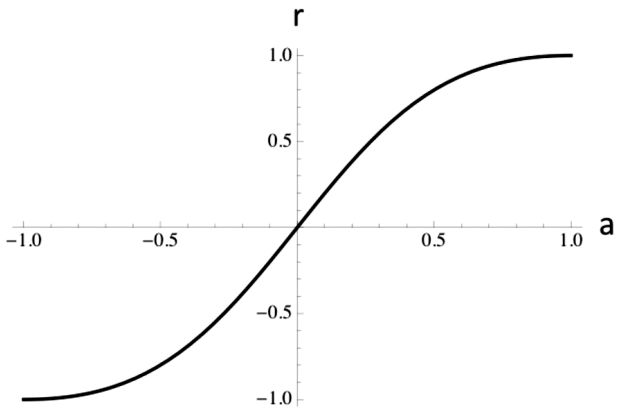

Fig. 2. Pearson correlation of the two classical oscillators coordinate as a function of the initial position of one of the oscillators ($x_1(0) = 1, \dot{x}_1(0) = 0, \dot{x}_2(0) = 0$ and $x_2(0) = a$, no friction and no driving).

We conclude that in this simple classical system, the synchronization level *r* (measured through the Pearson correlation) of the oscillators depends only on their initial relative phases and does not depend on any other physical parameters of this system. There is no phase-locked synchronization, unless the oscillators start completely in-phase or completely in anti-phase. The universal $r(a)$ curve is plotted in Fig. 2.

QUANTUM OSCILLATORS

The Hamiltonian operator of the corresponding quantum mechanical system writes as:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} - \frac{\hbar^2}{2M}\frac{\partial^2}{\partial x_3^2} + \frac{1}{2}k(x_1 - x_3)^2 + \frac{1}{2}k(x_2 - x_3)^2 \quad (7)$$

In order to study the evolution of this system, we make the assumption that all three masses start in the beginning as independent quantum oscillators initialized using their ground states wave functions centered around the mean coordinates: $\langle x_1 \rangle = x_{01}, \langle x_2 \rangle = x_{02}$ and $\langle x_3 \rangle = x_{03}$, respectively. The wave function of such system would be $\Psi_0(x_1, x_2, x_3) = \Psi_{01}(x_1)\Psi_{02}(x_2)\Psi_{03}(x_3)$, where

$$\Psi_{01}(x_1) = \left(\frac{\sqrt{mk}}{\pi\hbar}\right)^{\frac{1}{2}} \exp\frac{\sqrt{mk}(x_1 - x_{01})^2}{2\hbar}$$

$$\Psi_{02}(x_2) = \left(\frac{\sqrt{mk}}{\pi\hbar}\right)^{\frac{1}{2}} \exp\frac{\sqrt{mk}(x_2 - x_{02})^2}{2\hbar} \quad (8)$$

$$\Psi_{03}(x_3) = \left(\frac{\sqrt{Mk}}{\pi\hbar}\right)^{\frac{1}{2}} \exp\frac{\sqrt{Mk}(x_3 - x_{03})^2}{2\hbar}$$

This initial wave function can be represented as a linear combination of the eigenstates Ψ_n of the Hamiltonian (7):

$$\Psi_0(x_1, x_2, x_3) = \sum_n C_n \Psi_n(x_1, x_2, x_3) \quad (9)$$

The coefficients C_n are given as:

$$C_n = \iiint \Psi_n^*(x_1, x_2, x_3)\Psi_0(x_1, x_2, x_3)dx_1 dx_2 dx_3 \quad (10)$$

Now that we can represent the initial wave form as a combination of eigenstates, we can calculate the evolution of the system using the eigenstates Ψ_n and energy eigenvalues E_n

$$\Psi(x_1,x_2,x_3,t) = e^{-i\hat{H}t}\Psi_0(x_1,x_2,x_3) = \sum_n C_n \Psi_n(x_1,x_2,x_3)e^{-iE_n t} \tag{11}$$

In order to obtain the correlation between the coordinates of the two masses m, we must find the expectation values of x_1 and x_2:

$$\left\langle x_i(t)\right\rangle_\Psi = \iiint \Psi^*(x_1,x_2,x_3,t)x_i\Psi(x_1,x_2,x_3,t)dx_1dx_2dx_3 \tag{12}$$

We will treat the expectation values as equivalent to classical coordinates of the system. Similarly with the classical system, we choose the Pearson correlation coefficient as a measure of synchronization between the oscillators. In this approach the quantum mechanically computed order parameter is:

$$r = \frac{\left\langle X_1X_2\right\rangle_t - \left\langle X_1\right\rangle_t\left\langle X_2\right\rangle_t}{\sqrt{\left\langle X_1^2\right\rangle_2 - \left\langle X_1\right\rangle_t^2}\sqrt{\left\langle X_2^2\right\rangle_2 - \left\langle X_2\right\rangle_t^2}} \tag{13}$$

where $X_i = \left\langle x_i(t)\right\rangle_\Psi$ is obtained from (12). For an alternative calculation instead of this semi-classical Pearson correlation, one could use one where all the averages are quantum mechanically calculated

$$r' = \frac{\left\langle\left\langle x_1x_2(t)\right\rangle_\Psi\right\rangle_t - \left\langle X_1\right\rangle_t\left\langle X_2\right\rangle_t}{\sqrt{\left\langle\left\langle x_1^2(t)\right\rangle_\Psi\right\rangle_t - \left\langle X_1\right\rangle_t^2}\sqrt{\left\langle\left\langle x_2^2(t)\right\rangle_\Psi\right\rangle_t - \left\langle X_2\right\rangle_t^2}} \tag{14}$$

with:

$$\begin{aligned}\left\langle x_1x_2(t)\right\rangle_\Psi &= \iiint \Psi^*(x_1,x_2,x_3,t)x_1x_2\Psi(x_1,x_2,x_3,t)dx_1dx_2dx_3\\ \left\langle x_i^2(t)\right\rangle_\Psi &= \iiint \Psi^*(x_1,x_2,x_3,t)x_i^2\Psi(x_1,x_2,x_3,t)dx_1dx_2dx_3\end{aligned} \tag{15}$$

In our calculations we used classical averages for $\left\langle x_1x_2(t)\right\rangle$ and $\left\langle x_i^2(t)\right\rangle$, as quantum mechanical averages calculated from (15) coincide very closely with the classical averages for this system, yet bring in extra error due to the integration.

NUMERICAL APPROACH TO THE QUANTUM MECHANICAL PROBLEM

The first task is to obtain the eigenvalues and eigenvectors for the Hamiltonian (7). For this, we have to solve the stationary Schrödinger equation in three dimensions, which can be done only numerically. The simplest way to do

this is to confine the problem into a three-dimensional box where each spatial dimension of length L is represented by N equidistant points. This way we view the coordinate space as a three dimensional grid and we seek the solution for the nodes of this grid. As the grid is finite and uniform, instead of using three coordinates for the nodes of the grid, we can use only one index n ranging from 1 to N^3, which allows us to treat the wave function in this space as a one dimensional vector:

$$\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \dots \\ \Psi_n \end{pmatrix} \tag{16}$$

The global index n replaces the three oscillator coordinate indices i_{x_1}, i_{x_2} and i_{x_3} in such a way that the resulting one dimensional vector Ψ can later be restored into its three dimensional form in the following way:

$$\Psi(x_1, x_2, x_3) = \Psi_{x_1 + x_2 N + x_3 N^2} \tag{17}$$

In such case the coordinates x_1, x_2, x_3 can be obtained as:

$$\begin{aligned} x_1 &= n \bmod N \\ x_2 &= (n \text{ quotient } N) \bmod N^2 \\ x_3 &= n \text{ quotient } N^2 \end{aligned} \tag{18}$$

On this equidistant grid the second order derivatives can be calculated using the following three-point formulas

$$\begin{aligned} \frac{\partial^2 \Psi}{\partial x_1^2} &= \frac{\Psi_{n+1} - 2\Psi_n + \Psi_{n-1}}{\left(\frac{2L}{N+1}\right)^2} \\ \frac{\partial^2 \Psi}{\partial x_2^2} &= \frac{\Psi_{n+N} - 2\Psi_n + \Psi_{n-N}}{\left(\frac{2L}{N+1}\right)^2} \\ \frac{\partial^2 \Psi}{\partial x_3^2} &= \frac{\Psi_{n+N^2} - 2\Psi_n + \Psi_{n-N^2}}{\left(\frac{2L}{N+1}\right)^2} \end{aligned} \tag{19}$$

Thus, we can write the Hamiltonian as a $N^3 \times N^3$ matrix, and the Schrödinger equation as a matrix eigenproblem:

$$\sum_{j=1}^{N^3} H_{ij} \Psi_j = E \Psi_i \tag{20}$$

which can be solved by a standard algorithm using for example the Mathematica software.

After we've obtained the eigenvectors, we can transform them back into the three dimensional form. Using the initial states (8), the evolution of the system can be calculated according to (11) and (10). Naturally in equation (10) we replace the integrals with sums according to the used numerical integration algorithm.

COLLECTIVE BEHAVIOR IN THE QUANTUM MECHANICAL SYSTEM

In order to apply the numerical method to the quantum system, we need to establish the units for all variables. For convenience of the calculations we choose a system where $\hbar = 1$. The simulated space is a cube with side up to $N = 40$. The masses of the oscillators are equal, $m_1 = m_2 = m$, the spring constants are also equal, $k_1 = k_2 = 1$, and the platform's mass is fixed at $M = 1$.

With these values we can simulate the evolution of the system, as shown in Fig. 3. Note that the initial Gaussian wave packet disperses over time due to the coupling of the oscillators. However, this dispersion still allows for treating the wave function as a packet. The expectation values of $x_1(t)$ and $x_2(t)$ according to (12) are essentially coordinates that we can treat as classical positions of the oscillators for the purpose of calculating the degree of synchronization. As an example a particular time-evolution for these quantities is given in Fig. 4.

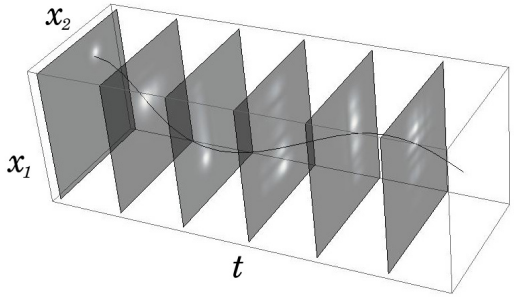

Fig. 3. Evolution of the system's wave function in the x_1, x_2 coordinate plane. The line is the trajectory of the expectation value of the system's coordinates.

As we are interested in the following in the dependence of the degree of synchrony on the initial positions of the oscillators, for computational convenience we fixed the initial position of one of the oscillators at $x_{01} = 1$ and vary that of the other oscillator's initial position between −1 and 1.

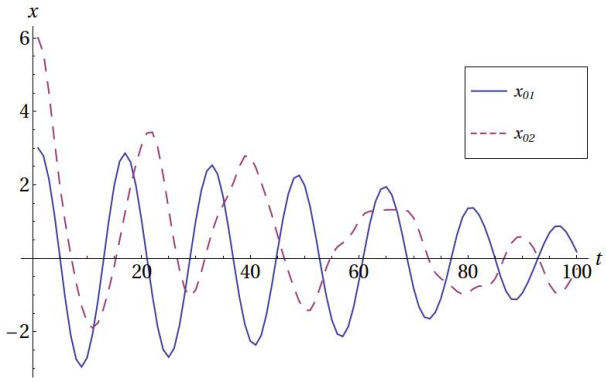

Fig. 4. Trajectories of the expectation values of x_1 and x_2 calculated with initial positions $x_{01} = 3$ and $x_{02} = 6$. The decrease in amplitude is due to the dispersion of the wave function.

Finite size effects due to the discretization of the space has a minimal influence on the obtained results. This is nicely visible on Fig. 5, where for $m = 1$ we present the computed Pearson-type correlation for different discretization $(N = 10;30;40)$. This result suggests, that $N = 40$ is an acceptable discretization, and such system sizes could still be handled by our Mathematica code.

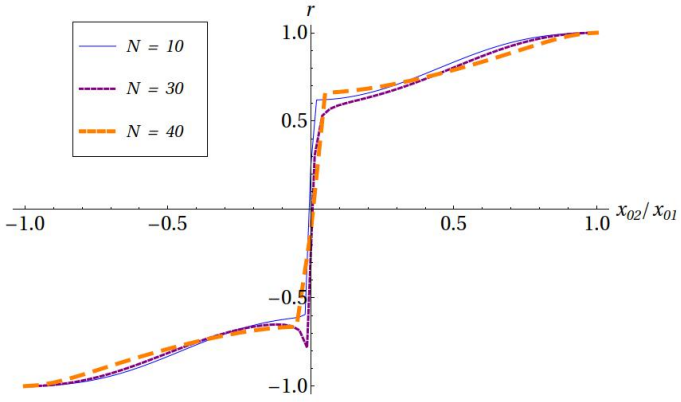

Fig. 5. Correlation curves with varying discretization number N and $m = 1$

On Fig. 6 we present the results for the correlation parameter as a function of the initial position of one of the oscillators, considering different m values. The observable trends are rather similar with the classical case: the oscillators move in a synchronicity if they start from similar coordinates and the motion is in anti-synchrony if they start in anti-phase. Beside this general trend, there are however visible differences between the quantum-mechanical and the classical curve. The collective behavior of the quantum-mechanical system is highly dependent on the mass ratio between the platform and the oscillators, whereas the classical system does not depend on it at all. In the quantum mechanical system, for small *m* values there is a large jump in the order parameter in the vicinity of the $x_{02} = 0$ point. Transition from the synchronized to anti-synchronized dynamics is much steeper, which means that the correlated and anti-correlated trends are much more pronounced in the quantum-mechanical system. This means, that even for a small amount of synchrony in the initial state, the system will move in a largely synchronous manner. The same is true for the initially anti-synchronized states.

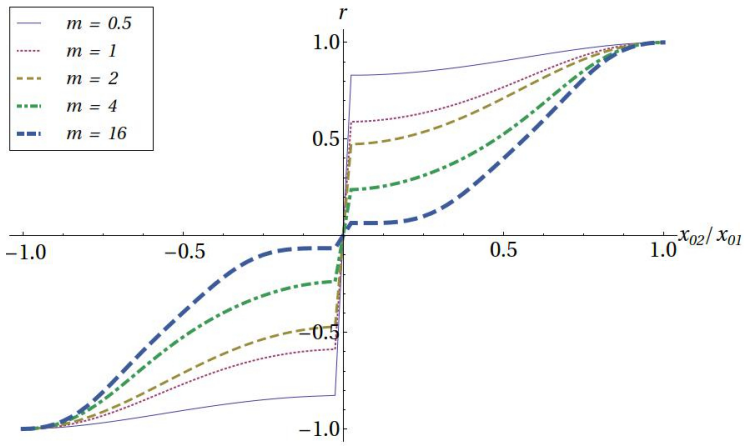

Fig. 6. Pearson correlation as a function of the initial position of one of the oscillators. Results for different m values and $N = 40$.

CONCLUSIONS

Unlike the classical system of coupled oscillators, which can be solved exactly, the quantum mechanical system could be handled only by numerical approximations. The presented results could be affected thus by border artifacts and other numerical errors. In spite of such limitations of the results, we feel that several interesting conclusions can be drawn.

First, we observed that the quantum mechanical system behaves much like the classical one in terms of the overall results regarding the initial positions of the oscillators: we obtained a collective behavior resembling synchrony if the oscillators start from similarly oriented displacements and a dynamics resembling anti-synchrony if they started from oppositely oriented initial positions. In difference with the classical coupled oscillator system, in the quantum mechanical system the transition between the positively and negatively correlated states (synchrony and anti-synchrony) is much sharper when the mass of the oscillators (m) is not too large relative to the mass of the coupling platform (M). In this limit the results indicate that the level of correlations and anti-correlations are more pronounced, which means that the quantum-mechanical system exhibits a stronger and more stable collective behavior than its classical counterpart. A noticeable difference relative to the classical system is the dependence of the observed trends as a function of m/M.

ACKNOWLEDGEMENT

We acknowledge support from research grant PN-II-ID-PCE- 2011-3-0348.

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