

Quantum gears: a simple mechanical system in the quantum regime

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Abstract. The quantum mechanics of a simple mechanical system is considered. A group of gears can serve as a model for several different systems such as an artificially constructed nanomechanical device or a group of ring molecules. An expression is derived for the quantisation of the dynamics of a 2-gear system. The general solution for several gears is discussed.

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1. Introduction

With the rapid rise in interest in micro- and nano-mechanical and electromechanical devices it will soon be necessary to consider the quantum aspects of the behaviour of such mechanical devices in the same way as the development of micro- and nano-scale electronic devices forces us to consider quantum finite size and interference effects as well as single electron effects (Drexler 1992, Cleland & Roukes 1999, Cleland 2002). As a model system to investigate the sort of effects which the onset of quantum behaviour could give rise to, a system of gears is considered. Such a system is a vital component of most classical “machines” but one for which it is easy to anticipate different behaviour in the quantum system. Classically the angular velocities of the gears are locked together by the action of the teeth, whereas in the quantum system the angular momenta of the individual gears will be quantised in a way which is not necessarily consistent with the expected classical solution.

The system of 2 gears serves as a model system for any nano-machine in which circular (or spherical components) are constrained to rotate at angular frequencies which have a fixed ratio to each other, but are also subject to quantisation of their angular momenta. One could consider, for example, anything involving different sized wheels moving along a surface, such as a “penny-farthing” bicycle.

For 2 gears with n_1 and n_2 teeth their angular velocities, ω_1 and ω_2 , are locked together as $n_1\omega_1 + n_2\omega_2 = 0$. On the other hand each of them is subject to an angular momentum quantisation, $L = I\omega = m\hbar$ where I is the moment of inertia and m is an integer. By eliminating the 2 ω 's we obtain a constraint on the behaviour of the pair of gears

$$n_1m_1I_1^{-1} = n_2m_2I_2^{-1} \quad (1)$$

which has no non-trivial solutions (i.e. with integer m_1 & m_2 other than $m_1 = m_2 = 0$) except for special cases such as 2 identical gears. The gears appear to be locked together such that they cannot rotate.

Is this picture too naïve? It must be possible to return to the classical behaviour as the gears become larger; somehow the gears must be unlocked on macroscopic scales. On the other hand there are lots of examples of systems with quantised angular momenta for which the strict quantisation is lifted when the systems are combined, such as when 2 atoms form a molecule and the previously quantised atomic orbitals are hybridised.

2. A Model

In order to investigate the matter further we consider the simplest Hamiltonian which describes such a system

$$H = \frac{L_1^2}{2I_1} + \frac{L_2^2}{2I_2} + V(n_1\theta_1 + n_2\theta_2) \quad (2)$$

$$= \frac{1}{2I_1} \left(\frac{\hbar}{i} \frac{\partial}{\partial \theta_1} \right)^2 + \frac{1}{2I_2} \left(\frac{\hbar}{i} \frac{\partial}{\partial \theta_2} \right)^2 + V_0 v(n_1\theta_1 + n_2\theta_2) \quad (3)$$

where θ_n is the angle of the n th gear, $0 \leq \theta < 2\pi$, and $v(\theta)$ is a periodic function with period 2π with a single minimum with $v = 0$ and a single maximum with $v = 1$ in each period. V_0 is the amplitude of the potential which describes the interaction between the gears. When $V_0 \rightarrow \infty$ the gears are constrained such that $n_1\theta_1 + n_2\theta_2$ is constant, as required. It will be useful, however, to consider finite V_0 as well.

Equation (3) may be separated by changing to new variables

$$p = \frac{I_1}{n_1}\theta_1 - \frac{I_2}{n_2}\theta_2 \quad (4)$$

$$s = n_1\theta_1 + n_2\theta_2 \quad (5)$$

which represent the primary and secondary motion of the gears respectively. Here *primary* refers to the usual motion expected of gears in which the angular velocities have a fixed ratio and *secondary* refers to the deviation from the primary behaviour.

In terms of p and s the Hamiltonian may now be rewritten as

$$-\frac{\hbar^2}{2} \left(\frac{n_1^2}{I_1} + \frac{n_2^2}{I_2} \right) \frac{\partial^2}{\partial p^2} - \frac{\hbar^2}{2} \left(\frac{I_1}{n_1^2} + \frac{I_2}{n_2^2} \right) \frac{\partial^2}{\partial s^2} + V_0 v(s), \quad (6)$$

2.1. Classical behaviour

The part in p of (6) is the equation of a free system with an effective moment of inertia, I_{eff} , such that

$$\frac{1}{I_{\text{eff}}} = \frac{n_1^2}{I_1} + \frac{n_2^2}{I_2}. \quad (7)$$

The rest of (6) describes a system subject to the potential $V_0 v(s)$ whose behaviour depends on whether the energy is greater than or less than V_0 . For a classical system in the former case the motion is effectively free, whereas in the latter case the system oscillates around the minimum of the potential. Manufacturers of gears typically try to design the teeth to minimise this motion.

2.2. Quantum behaviour

What changes when we consider the quantum solutions of (6)? Firstly, the case $V_0 = 0$: here the solutions are simple plane waves in both representations and are subject to the boundary conditions that the wave function is single-valued and continuous at $\theta = 0, 2\pi$ giving

$$\exp(im_1\theta_1) \exp(im_2\theta_2) = \exp(k_p p) \exp(ik_s s). \quad (8)$$

Combining this with the definitions of p and s and demanding that the equation is valid for all (θ_1, θ_2) gives the quantisation conditions

$$k_p = \left(\frac{n_1 n_2}{I_1 I_2} (m_1 n_2 - m_2 n_1) \right) \left(\frac{n_1^2}{I_1} + \frac{n_2^2}{I_2} \right)^{-1} \quad (9)$$

$$k_s = \left(\frac{n_1 m_1}{I_1} + \frac{n_2 m_2}{I_2} \right) \left(\frac{n_1^2}{I_1} + \frac{n_2^2}{I_2} \right)^{-1} \quad (10)$$

When V_0 is finite the secondary part of (6) is identical to the Schrödinger equation for a 1-dimensional crystal as discussed in any textbook of solid state physics (Ashcroft & Mermin 1976). The particular results required here are

- (i) the matrix elements of the periodic potential with different wave-like solutions are non-zero only when the wave vectors are related by

$$k'_s = k_s + j. \quad (11)$$

In the present case the integral over p in the evaluation of the matrix elements is non-zero only for terms diagonal in k_p .

- (ii) it follows that k_s values in the range $-\frac{1}{2} < k_s \leq +\frac{1}{2}$ are good quantum numbers representing independent solutions (i.e. they are in the 1st Brillouin zone). k_p is always a good quantum number.
- (iii) the group velocity dE/dk_s , where E is the energy, is identically zero for $k_s = m\frac{1}{2}$ where m is an integer (i.e. at the middle and edges of the Brillouin zone).
- (iv) in the limit $V_0 \gg E$ the states in each unit cell are decoupled from one another and the group velocity tends to zero.

Using result (i) and (10) we can write

$$\frac{n_1 m'_1}{I_1} + \frac{n_2 m'_2}{I_2} = \frac{n_1 m_1}{I_1} + \frac{n_2 m_2}{I_2} + j \left(\frac{n_1^2}{I_1} + \frac{n_2^2}{I_2} \right) \quad (12)$$

It is useful to visualise this by considering vectors on a 2D rectangular lattice with basis vectors $(I_1^{-1/2}, I_2^{-1/2})$ so that (12) may be expressed as

$$\mathbf{m}' \cdot \mathbf{n} = \mathbf{m} \cdot \mathbf{n} + j \mathbf{n}^2 \quad (13)$$

where the vectors \mathbf{n} represent points on the lattice with the integer components (n_1, n_2) and the terms in (13) represent projections of the vectors onto \mathbf{n} . The simple solution of (13) for \mathbf{m}' is given by

$$\mathbf{m}' = \mathbf{m} + j \mathbf{n} \quad (14)$$

but other solutions may be found by adding a lattice vector perpendicular to \mathbf{n} . Note, however, that k_p contains $\mathbf{m} \times \mathbf{n}$ so that the addition of such a vector would change the value of k_p . Thus (14) is in fact the complete solution.

The general solution for the wave function of the two gear system can therefore be written as

$$\psi_{\mathbf{m}}(p, s) = \exp [ik_p(\mathbf{m})p] \sum_j a_j \exp [ik_s(\mathbf{m} + j\mathbf{n})s] \quad (15)$$

where the solutions are distinct for all \mathbf{m} not related by (14).

For hard gears ($V_0 \rightarrow \infty$) using (iv) above the group velocity of the secondary part is zero; the teeth of the gears do not tunnel through each other. Apart from the zero point energy of the secondary part the energy of the system may be written

$$E = -\frac{\hbar^2}{2} \left(\frac{n_1 n_2}{I_1 I_2} \right)^2 \left(\frac{n_1^2}{I_1} + \frac{n_2^2}{I_2} \right)^{-1} (m_1 n_2 - m_2 n_1)^2 \quad (16)$$

2.3. Soft gears

When V_0 is finite it becomes possible for the teeth of the gears to tunnel through one another. One might visualise this in terms of the interaction between 2 ring molecules where the effective value of V_0 would depend on their separation.

For such gears to be useful the group velocity of the secondary part should be zero, which from (iii) above can only be guaranteed for k_s at the centre and edges of the Brillouin zone, where k_s is an integer multiple of $\frac{1}{2}$ or

$$\mathbf{m} \cdot \mathbf{n} = \frac{j}{2} n^2. \quad (17)$$

When $I_1 = I_2$ and $n_1 = n_2$ there are many such solutions, but when $(I_1/I_2)^{1/2}$ is irrational there are none at all.

3. Many Gears — A Quantum Machine

We define a quantum machine as a collection of gears all interlocking with each other, either directly or indirectly, such that, classically, if one is rotating then all are. There are cases, such as 3 mutually interlocking gears, which are classically frustrated but which may have quantum solutions involving tunnelling of the teeth. Such systems will not be considered here.

An N -gear system will have a wave function which may be written in the form $\psi(p, s_1, \dots, s_{N-1})$ where

$$p = \sum_{i=1}^N a_i \theta_i \quad (18)$$

$$s_i = n_i \theta_i + n_{i+1} \theta_{i+1}. \quad (19)$$

The 2nd derivatives in the kinetic energy terms of the Hamiltonian may then be written as

$$\begin{aligned} \frac{\partial^2}{\partial \theta_1^2} &= \left(a_1 \frac{\partial}{\partial p} + n_1 \frac{\partial}{\partial s_1} \right)^2 \\ &\vdots \\ \frac{\partial^2}{\partial \theta_i^2} &= \left(a_i \frac{\partial}{\partial p} + n_i \frac{\partial}{\partial s_{i-1}} + n_i \frac{\partial}{\partial s_i} \right)^2 \\ &\vdots \\ \frac{\partial^2}{\partial \theta_N^2} &= \left(a_N \frac{\partial}{\partial p} + n_N \frac{\partial}{\partial s_{N-1}} \right)^2 \end{aligned} \quad (20)$$

For the p part of the equation to be separable the coefficients of the partial derivatives of the form $\partial^2/\partial p \partial s_i$ should be zero. This requires that

$$\frac{a_i n_i}{I_i} + \frac{a_{i+1} n_{i+1}}{I_{i+1}} = 0 \quad (21)$$

which has a solution

$$a_i = (-1)^i \frac{I_i}{n_i}. \quad (22)$$

Let us now assume that the general solution may be written in the form

$$\exp(ik_p p) f(s_1, \dots, s_{N-1}) = \sum_{m_1, \dots, m_N} c_{m_1, \dots, m_N} \prod_{i=1}^N \exp(im_i \theta_i) \quad (23)$$

such that the primary part may be separated and takes a simple wave form and the total function may be written as a sum over every possible rotational state of the gears.

The coefficient c for a particular set of m 's may be calculated using

$$(2\pi)^N c_{m_1, \dots, m_N} = \prod_i \int_0^{2\pi} d\theta_i \exp(-im_i \theta_i) \exp(ik_p p) f(s_1, \dots, s_{N-1}). \quad (24)$$

To evaluate this integral it is useful to transform it into the p and s_i representation by writing

$$\begin{bmatrix} p \\ s_1 \\ \vdots \\ s_{N-1} \end{bmatrix} = \begin{bmatrix} -(I_1/n_1) & (I_2/n_2) & \cdots & (-1)^N (I_N/n_N) \\ n_1 & n_2 & & \\ & \ddots & \ddots & \\ & & n_{N-1} & n_N \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_N \end{bmatrix} \quad (25)$$

$$\mathbf{p} = \mathbf{T}\boldsymbol{\theta}$$

so that the (24) becomes

$$c_{\mathbf{m}} \propto \int_{-\infty}^{+\infty} dp \prod_{i=1}^{N-1} \int ds_i \exp(-i \mathbf{m} \cdot \mathbf{T}^{-1} \mathbf{p}) \exp(ik_p p) f(s_1, \dots, s_{N-1}) \quad (26)$$

where \mathbf{m} and \mathbf{p} are vectors with components (m_1, \dots, m_N) and (p, s_1, \dots) respectively and we can extend the limits on the integral to $\pm\infty$ without loss of generality.

The integral over p in (26) is zero unless

$$k_p = \sum_i m_i [\mathbf{T}^{-1}]_{i1}. \quad (27)$$

In order to evaluate \mathbf{T}^{-1} consider the equation $\sum_j T_{ij} \tau_j = \delta_{i1}$. All but the 1st row may be rewritten

$$\tau_i = -\frac{n_{i-1}}{n_i} \tau_{i-1} = (-1)^{i-1} \frac{n_1}{n_i} \tau_1. \quad (28)$$

Substituting this into the 1st row gives

$$\sum_{i=1}^N (-1)^i \frac{I_i}{n_i} \tau_i = -\sum_{i=1}^N \frac{I_i}{n_i^2} n_1 \tau_1 = 1 \quad (29)$$

which leads to the result

$$\tau_i = \frac{(-1)^i}{n_i} / \sum_{j=1}^N \frac{I_j}{n_j^2} \quad (30)$$

and from (27)

$$k_p = \left(\sum_{i=1}^N (-1)^i \frac{m_i}{n_i} \right) / \left(\sum_{i=1}^N \frac{I_i}{n_i^2} \right) \quad (31)$$

Using (20) the kinetic energy of the primary motion of the system may be evaluated as

$$E = -\frac{\hbar^2}{2} \left(\sum_{i=1}^N \frac{I_i}{n_i^2} \right) \frac{\partial^2}{\partial p^2} \quad (32)$$

$$= \frac{\hbar^2}{2} \left(\sum_{i=1}^N (-1)^i \frac{m_i}{n_i} \right)^2 / \left(\sum_{i=1}^N \frac{I_i}{n_i^2} \right). \quad (33)$$

Compare these results with (9) and (16).

4. Conclusions

The quantum mechanics of a system of interlocking gears has been considered as a model for a nano-machine. It has been shown that the locking of the gears tentatively predicted in the introduction does not occur and an expression has been derived for the quantised energy of 2 gears. The case of N interlocking gears has been considered and a general expression for the quantisation of the primary motion has been presented.

When the potential describing the interaction of the teeth is softened most solutions involve tunnelling of the teeth.

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