In this section of *Resonance,* we invite readers to pose questions likely to be raised in a classroom situation. We may suggest strategies for dealing with them, or invite responses, or both. "Classroom" is equally a forum for raising broader issues and sharing personal experiences and viewpoints on matters related to teaching and learning science.

Getting Acquainted with Gears and Wheels – Quantum Mechanically

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For a pair of wheels or gears with positive coupling, i.e., without slip or play, there are rules of engagement that have some interesting consequences when their dynamics is treated quantum mechanically. We will illustrate the principal ideas involved here with the help of an elementary, basically a textbook exercise whose solution, however, is not only interesting, but may also be re-interpreted rather creatively. Possible relevance of this simple exercise to the incredible, ever-shrinking world of the nano (1 nm = 10^{-9} m) is pointed out.

1. Introduction and Motivation

The invention of the wheel has been considered by many to be one of the oldest and the greatest inventions of mankind, dating back to ca.1000 BC. The same may more are less, be said of the gear (*Figure* 1) – after all, the toothless wheel is an *analog* of the *digital* toothed gear.

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Nano-gears, no-slip condition, constraint, quantum mechanics.

For a mathematically minded number theorist, however, we hasten to add that the gear has a countable discrete-

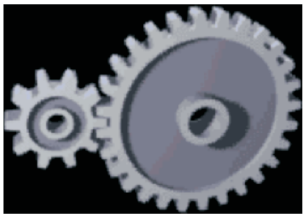

Figure 1. Two gears engaged so as to transmit motion.

ness, i.e., its teeth can be counted, whereas the wheel is an uncountable continuum. The twain have different cardinality! In the following, however, we will continue to use the two terms interchangeably. After all, for any wheel one can always find a gear approximant to the desired order of precision/resolution. Some of these issues will recur in the course of our discussion.

Over the millennia, natural philosophers (physicists and mathematicians) and engineers alike have engaged with the gear/wheel and the complex mechanisms based on these. In fact, Aristotle (ca. 300 BC) had suggested the use of the frictionally engaged wheels to transmit motion. Some of the other great names that readily come to the mind are Archimedes (ca. 250 BC) for his association with the design of the *antikythera* – a geared mechanical computer of great complexity; Galileo (ca. 1600 AD) for the *Galilean Jovilabe* with the surprising *non-reversibly* geared clock mechanism; and so on until we finally come to James Clerk Maxwell (1837–1879), who created a truly powerful mental construct, a mechanical model for the electromagnetic phenomena – with tiny spinning cells, idler wheels, and roller contacts without slip, filling the space [1].

We have, of course, come a long way – from the potter's crude wooden wheels to the finely geared watches and the robust power machines – and we see gears at every turn of an engine. But, no matter how sophisticated and varied are our gears today as compared to the potter's ancient wheels, they all share a basic commonality – they are all governed by classical mechanics (Newton's Laws of Motion). But, this may have to change now as we continually downsize our devices to the nano/sub-nanoscales; and still there seems to be plenty of room left at the bottom [2]. A question one may reasonably ask now is whether these enmeshed nano-gears will behave essentially in the same manner as the gears we are familiar with. Well, the answer is a definite NO!

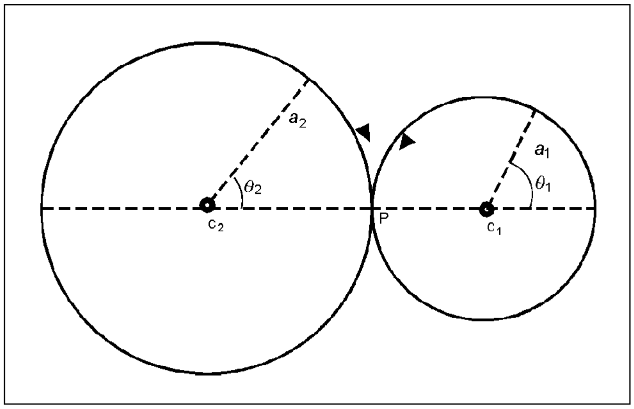

Figure 2. Two engaged wheels without slip; analog version of the enmeshed digital gear.

The domain of the nano/sub-nanoscale is ruled by the quantum. There may be surprises and even some creative re-interpretations possible. We must, therefore, get re-acquainted with the gear and the wheel – but now quantum-mechanically! And we will do this here through a study of the simplest of examples, viz., a pair of coupled circular discs lying in a plane.

Consider a system of two co-planar discs 1 and 2 of radii a_1 and a_2, free to rotate about their respective centres c_1 and c_2 fixed in the plane, and *enmeshed* such that there is no slip at the point of their contact P as shown in *Figure* 2. This schematic depicts our elementary model system of two wheels/gears properly engaged.

A *classical* treatment of this two-body dynamical system begins with the Lagrangian, $L = K - U$ for the system, where K is its total kinetic energy expressed in terms of the (angular) velocities $\dot{\theta}_1$ and $\dot{\theta}_2$, and U is the total potential energy as a function of the (angular) coordinates θ_1 and θ_2. Inasmuch as there is no energy term depending on the (angular) coordinates θ_1 and θ_2, the total potential energy $U = 0$. Now, the total kinetic energy (K) of the coupled system is given by

$$K = \frac{1}{2}I_1\dot{\theta}_1^2 + \frac{1}{2}I_2\dot{\theta}_2^2 \tag{1}$$

with $I_1(=\frac{1}{2}M_1a_1^2)$ and $I_2(=\frac{1}{2}M_2a_2^2)$ being the moments of inertia of the two circular discs of mass M_1 and M_2 respectively. Here the overhead dot denotes time derivative.

Next, we turn to the no-slip constraint. This may be implemented through the condition

$$a_1\dot{\theta}_1 = -a_2\dot{\theta}_2. \qquad (2)$$

The classical dynamics is, therefore, completely determined by the total kinetic energy K and the no-slip constraint, as in (1) and (2) respectively. (A classical dynamical system with constraints involves, in general, somewhat advanced methods of classical mechanics [3]. Further, the presence of any angle-dependent potential would have made the no-slip condition non-trivial to implement). In the present case, however, we can simply rewrite the constraint in equation (2) as,

$$\dot{\theta}_2 = -\left(\frac{a_1}{a_2}\right)\dot{\theta}_1, \qquad (3)$$

and thus eliminate $\dot{\theta}_2$, say, in favour of $\dot{\theta}_1$ throughout. (Clearly, we could equally well eliminate $\dot{\theta}_1$ in favour of $\dot{\theta}_2$, and then repeat the same treatment as given below. We will obtain the same final results. The reader is encouraged to verify this explicitly). We can now express the kinetic energy K given in (1) as a function of $\dot{\theta}_1$, alone:

$$K = \frac{1}{2}\left[I_1 + I_2\left(\frac{a_1}{a_2}\right)^2\right]\dot{\theta}_1^2 \equiv \frac{1}{2}I\dot{\theta}_1^2 \qquad (4)$$

with I an *effective* moment of inertia. Thus, the no-slip constraint in (2) has effectively reduced the number of degrees of freedom by one (without changing the physics, of course). For the sake of clarity, let us rename this remaining degree of freedom as $\phi(\equiv \theta_1)$. Since, as noted above, there is no potential energy term in this problem, the kinetic energy K expressed entirely in terms of the angular velocity $\dot{\theta}_1(\equiv \dot{\phi})$ is nothing but the total Lagrangian L for the system.

Next, we go from the Lagrangian (L) to the Hamiltonian (H) which is convenient for treating the problem quantum mechanically. For this, we have to introduce the canonical (angular) momentum J *conjugate* to the (angular) coordinate ϕ as

$$J = \frac{\partial L}{\partial \dot{\phi}} = I\dot{\phi}. \tag{5}$$

The classical Hamiltonian H is then given by the Legendre transformation $H = J\dot{\phi} - L$, and expressing the latter in terms of the canonical momentum J using (5). We at once obtain [3]

$$H = \frac{J^2}{2I}. \tag{6}$$

This essentially completes the classical Hamiltonian formulation of the 2-disc problem with the no-slip constraint built in. It is to be noted that equation (6), together with (5), describes effectively a *single*-disc problem, with the effective disc moment of inertia $= I$. This is classically exact in and of itself. Here J is the constant of motion related to the conserved energy ($= J^2/2I$) of the system. We would like to re-emphasize here that in a classical mechanical treatment, the two-disc problem with no-slip condition is mathematically completely equivalent to a one-disc problem; i.e., from their classical dynamical (Newtonian) equations of motion, one cannot tell the two apart. As will be shown below, this, however, is not the case quantum-mechanically, and the physics becomes rather subtle.

Let us, therefore, turn now to a quantum treatment of the same two-disc problem. Note first that in the classical case as treated above, the existence of the other disc (disc 2) is, of course, implicit – but it enters only parametrically in the effective one-disc Hamiltonian as a modified moment of inertia (equation (6)). In the quantum-mechanical treatment too, the Hamiltonian formally appears as in the one-disc problem, but the mere existence of the (now *hidden*) other disc in the original two-disc problem brings about certain global changes in the allowed solutions that have observable consequences – quantitatively as well as qualitatively. Let us see how this comes about.

In the quantum case, the classical Hamiltonian H and the angular momentum J as derived above are to be treated as operators ($\hat{H}$ and $\hat{J}$), with

$$\hat{H} = \frac{\hat{J}^2}{2I}, \quad \text{and} \quad \hat{J} = -i\hbar\frac{\partial}{\partial\phi}, \tag{7}$$

whose eigenvalues give the simultaneously allowed energy and the angular momentum for the 2-disc dynamical system. (Note that $\hat{H}$ and $\hat{J}$ are Hermitian operators with real eigenvalues, and they commute). All we have to do now is to solve the associated eigenvalue equation (the time-independent Schrödinger equation)

$$\hat{H}\psi(\phi) \equiv -\frac{\hbar^2}{2I}\frac{\partial^2\psi(\phi)}{\partial\phi^2} = E\psi(\phi), \tag{8}$$

where we have explicitly indicated the (angular) coordinate ϕ as the argument of the wavefunction $\psi(\phi)$. (Recall that $\phi \equiv \theta_1$). The solution is readily seen to be

$$\psi(\phi) \propto e^{ik\phi} \quad \text{(to within a normalization)} \tag{9a}$$

with

$$E_k = \frac{\hbar^2 k^2}{2I} \quad \text{(the energy eigenvalue)}, \tag{9b}$$

where the parameter k is to be determined from the boundary condition for the problem as follows.

Formally, (9) may well describe a one-disc problem with an effective moment of inertia $\left(I_1 + I_2(a_1/a_2)^2\right)$. For such a one-disc problem, the single-valuedness of the wavefunction would demand a periodic boundary condition with period 2π, i.e., $\psi(\phi) = \psi(\phi + 2\pi)$ inasmuch as for the single disc, the angles ϕ and $\phi + 2\pi$ refer to identical single-disc configurations (i.e., a complete cycle, or a 2π-turn restores the disc to *status quo ante*!). The periodic boundary condition $e^{ik2\pi} = 1$ then forces k to be an integer (= N, say) giving the allowed energy eigenvalues as $E_N = \frac{\hbar^2 N^2}{2I}$. This result is, however, *not valid* in the quantum two-disc case inasmuch as the two enmeshed sub-systems, namely the two discs, must be treated as *a single whole system* with a *global wavefunction*. The uniqueness of this global wavefunction, therefore, demands that any two configurations of the two-disc system be now *identified* as being the *same* if they differ by integral numbers (n_1 and n_2, say) of complete turns of the two component discs 1 and 2. This leads to a novel strictly quantum mechanical feature, as discussed below.

The no-slip condition now constrains $\mid n_1 a_1 \mid = \mid n_2 a_2 \mid$ with a_1 a_2, say, without loss of generality. Clearly, this can be satisfied if and only if the wheel ratio a_1/a_2 = a rational number. (This is quite analogous to the problem of periodic occurrences (*syzygy*) of straight-line alignment of planets in our solar system, the period being essentially the lowest common multiplier (LCM) of the planetary periods). Thus, in our case, for example, if $a_1/a_2 = 4/6 \equiv 2/3$, then 3 turns of disc 1 will correspond to 2 turns of disc 2. So, for this case, the single-valuedness of the global wavefunction requires $k \times 3 \times 2\pi = N \times 2\pi$, or $k = N/3$, giving $E_N = \frac{\hbar^2}{2I}\left(\frac{N^2}{9}\right)$ as the allowed energy eigenvalues, where the energy-level index N is an integer. For the general case of rational wheel ratio, therefore, the energy eigenvalues E_{N} turn out to be given by

$$E_N = \frac{\hbar^2 N^2}{2I n_1^2}, \qquad (10)$$

where the wheel ratio $a_1/a_2 = n_2/n_1$, and the integers n_2 and n_1 are without common factors (relatively prime).

For gears, the gear ratio is clearly a rational number and the above treatment goes right through. But, on the other hand, for the case of two discs the wheel ratio (analogue of the gear ratio) can be irrational. For this case, we cannot find integers n_1, n_2 such that $| n_1 a_2 | = | n_2 a_2 |$, as required by the no-slip (constraint) condition. Then the above scheme of quantization clearly fails. It is, however, still possible to construct physically sensible solutions for the rational wheel-ratio approximants to a desired order of precision. Thus, e.g., for the wheel ratio $a_1/a_2 = 1/\sqrt{2}$, with

$$\sqrt{2} = 1.41421 \quad 35623 \quad 73095 \quad 04880 \quad 16887$$
$$24209 \quad 69807 \cdots ,$$

clearly an irrational number, we can construct rational approximants for $\sqrt{2}$ to increasing orders of precision, namely $\frac{14}{10}, \frac{141}{100}, \frac{1414}{1000} \cdots$. (Note that these rational approximants have to be listed out in long hand – there is no shortcut to the approximant of a given order).

In *Figure* 3, we have plotted semi-logarithmically the dimensionless energy-level values $e_N \equiv (2I/\hbar^2)E_N$ vs the

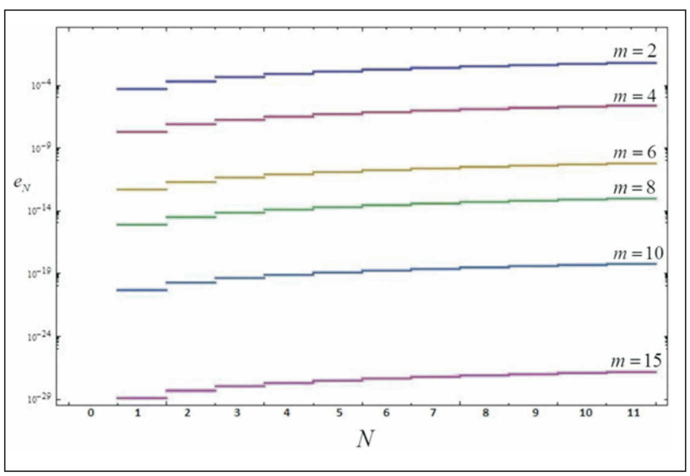

Figure 3. Energy spectrum for a two-disc system having irrational wheel ratio (ration of radii). Semi-log plot of dimensionless level energy $E_N \equiv E_N(2I/\hbar^2)$ vs the level index *N* for different orders *m* of the rational approximant.

energy-level index N for various orders (m) of the rational approximants. As can be readily seen, the energy levels tend to a continuum as m tends to infinity, which is to be expected physically.

It is interesting to note that the above treatment of the no-slip two-disc system can be readily extended to the case of many discs coupled without slip, e.g., a system including a number of idlers.

Let us provoke the still interested reader with a tempting generalization in which our *two discs* are now replaced with *two spheres*, as shown in *Figure* 4, free to turn about their fixed centres c_1 and c_2, but again under the no-slip rule of engagement. Now, however, the no-slip constraint operates entirely differently – thus, arbitrary rotations of the two spheres about the common z-axis passing through their centres c_1 and c_2, subtend no linear velocities in the common tangent plane normal to the $c_1 - c_2$ axis at the point of contact P, i.e., the no-slip constraint is trivially satisfied. On the other hand, for rotations about other orthogonal axes, this is not the case and the no-slip condition has to be imposed non-trivially. One has to go to some convenient coordinate system to simplify the calculation.

Quantum-mechanically, there is an added complication too – while classically, infinitesimal rotations commute, quantum mechanically they do not. This is expected to

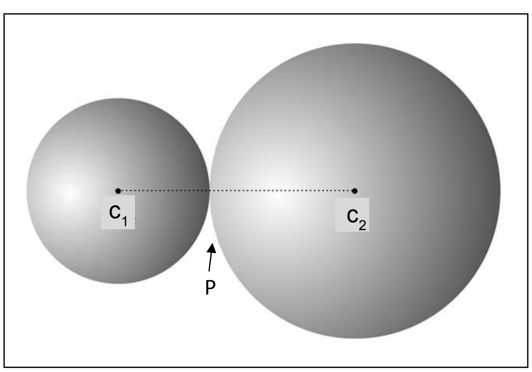

Figure 4. Two engaged spheres free to rotate about their centres without slip.

make the two-sphere case very different from its two-disc counterpart when the problem is treated quantum mechanically.

The whole point really is that the other (*hidden*) disc/sphere shows up very differently in the classical and the quantum cases. Thus, in the classical case, the hidden disc/sphere affects the effectively single-disc/sphere problem through a mere modification of the parameters occurring in its energy expression. (This is quite analogous to the case of the *invisible* Neptune showing up as causing a visible deviation of Uranus from its otherwise expected orbit). In the quantum case, however, the no-slip constraint enters qualitatively differently through the requirement of single-valuedness of the global wavefunction for the whole system. Thus, the effect of the other, *hidden* disc/sphere, admits a possible re-interpretation in terms of an effective one-disc/sphere system as being a *new elementary object in its own right*, e.g., in the case of the two-sphere system, the new object may have a different, even fractional, angular momentum! The interested reader is encouraged to explore this rather subtle point further – the unreasonable effectiveness of the *hidden* variable!

Finally, quantum wheels and gears are to be viewed in the present context of the fast emerging world of the nano [6]. *Figure* 5 demonstrates the idea of a molecular-scale train of nano-gears, 1.2 nm across and a few atoms

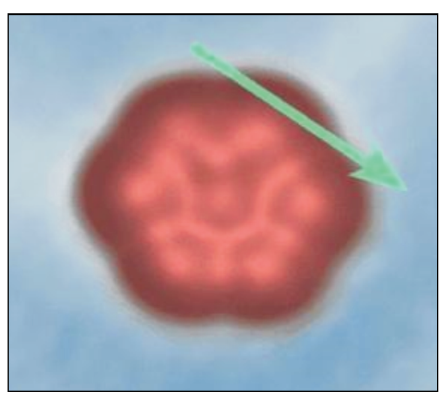

Figure 5. Working molecular nano-gear 1.2 nm across and a few atoms wide. From [7].

wide already made, or rather synthesized in the laboratory [7]. The possibility of realizing other machine components, like nano-rods, axles, van der Waals bearings, and the σ-bond based hinges for the nano, indeed organic-molecular scales, seems quite realistic now. Quantum wheels and gears will make us re-think many other physical aspects of the nano – such as friction and lubrication on the nanoscale. The high surface-to-volume ratio should, for example, help us with the heating problem.

We would like to conclude this conversational classroom exercise on the note that it is time now to *gear* up to the challenges of the nano – quantum mechanically!

Suggested Reading

[1] For a thoughtful account of Maxwell's creative ideas on a mechanical model, with spinning cells, idler wheels and roller contacts without slip, for the electromagnetic phenomena, see Basil Mahon, *The Man Who Changed Everything: The Life of James Clerk Maxwell*, John Wiley, 2003.

[2] R P Feynman, There is plenty of room at the bottom, *Caltech Engg. & Science*, Vol.23, pp.22–36, 1960. Available at http://www.zyvex.com/nanotech/feynman.html.

[3] H Goldstein, *Classical Mechanics*, Reading, Mass., Addison-Wesley Publishing Co. Inc., 1950.

[4] D J Griffiths, *Introduction to Quantum Mechanics*, V Edition, Prentice-Hall of India, New Delhi, 2006.

[5] C Kittel, *Introduction to Solid State Physics*, Wiley Eastern University Press, New Delhi, 1977. Also, see Angus Mackinnon, arXiv: cond-mat/ 020 5647

[6] NANO, *The Emerging Science of Nanotechnology*, Little, Brown and Company, London, 1995.

[7] See *ScienceDaily*, June 15, 2009. http://www.sciencedaily.com/releases/2009/\\06/090615102036.htm