AAPT PHYSICS EDUCATION | AMERICAN JOURNAL of PHYSICS

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Citation: American Journal of Physics **31**, 161 (1963); doi: 10.1119/1.1969339
View online: http://dx.doi.org/10.1119/1.1969339
View Table of Contents: http://scitation.aip.org/content/aapt/journal/ajp/31/3?ver=pdfcov
Published by the American Association of Physics Teachers

Quantum Mechanics of Beats between Weakly Coupled Oscillators*

PAUL H. E. MEIJER AND TOMOYASU TANAKA
The Catholic University of America, Washington, District of Columbia
(Received 9 August 1962)

Although the weakly coupled double pendulum seems to be a standard illustration in classical mechanics, it is seldom mentioned in quantum mechanics. It shares this fate with the damped harmonic oscillator, but while there is a good reason for avoiding the last one in quantum mechanics, the first can be treated with the same procedure as in classical mechanics. The exact solution is then compared with the solutions obtained by time-independent and time-dependent perturbation methods. It turns out that there are some additional steps to be taken, compared to the usual textbook treatment of the time-independent perturbation theory, due to the fact that all the levels of the unperturbed problem are degenerate. It is shown that the diagonalization of the secular matrix in the time-independent problem is equivalent to a problem of rotation of angular momentum operators in function space. The time-dependent problem needs, again, additional steps due to the degeneracy, and it yields the well-known beat-behavior.

THE basic idea of many linear problems in mathematical physics is the recognition of the normal modes of the problem. In its simplest form, this is illustrated with the double pendulum which shows the basic characteristics of nearly all linear problems in mathematical physics: the initial condition has to be decomposed in normal modes and the solution for $t>0$ is determined by these amplitudes and certain time constants which are found from the diagonalization of a matrix.

Since one can illustrate many features of quantum mechanical time-dependent perturbation theory with the help of this simple system it is worthwhile to display the solution of this problem in quantum mechanics. The calculation can be performed in three different ways. First, one can solve the problem exactly by diagonalization of the potential energy. This is done in the first section. Second, one can consider this model as an illustration for the (time-independent) perturbation theory by assuming that one has two independent oscillators with a weak mutual interaction. Finally, this model will serve to illustrate time-dependent perturbation theory. We take two independent oscillators, the first one in an excited state, the second in the ground state. At time $t=0$ we introduce suddenly the interaction potential and watch the behavior of the first oscillator.

All this follows standard methods and no new results are obtained. The energy which was originally concentrated in the first oscillator will transfer to the second oscillator in the same fashion as the classical problem behaves, as is the case with many other characteristics of the harmonic oscillator.[1]

The time-independent perturbation theory is performed in the standard fashion. We deal with a degenerate initial state, hence the secular matrix has to be diagonalized. At first sight this looks like a considerable task, at least for arbitrary n value, but the matrix turns out to be equivalent to one of the matrices in angular momentum theory, hence the eigenvalue can be obtained by a simple argument. It is amusing to see that the exact solution for the eigenvalues is much easier to obtain than the approximate solution.

The "test" of the time-dependent perturbation theory also brings out a rather interesting point. In this case the usual prescriptions do not work since both "initial" and "final" levels are degenerate and only one of the components of the "initial" level is occupied at $t=0$ in the initial value problem we are posing ourselves. The necessary modification, that is first to introduce the secular transformation on the level system before one applies the variation of constants techniques leads to the well-known beats of the double pendulum.

* Supported by the U. S. Air Force.

[1] We would like to use this opportunity to conjecture a new "theorem": All suggestions about the similarity between quantum mechanical and classical mechanics which are the result of the harmonic oscillator problem are not true in general!

There is an interesting application of this model known for a long time. It was noticed by Fermi in 1931[2] that in a CO_2 molecule the first level of the symmetric stretching mode has approximately the same frequency as the second level of the bending mode. Later, this phenomenon was found also in a number of similar molecules. The details of this situation differ. First, the coupling is not of the type x_1x_2 but proportional to $x_1x_2^2$ since lower monomials are excluded by symmetry arguments. Secondly, the oscillator number two is actually a two-dimensional oscillator, which introduces a degeneracy already in the uncoupled problem. Thirdly, as mentioned before, the "bare" frequencies are not comparable ($\nu_1 \approx \nu_2$) but one is double the other $\nu_1 \approx 2\nu_2$. This will make a complete calculation more elaborate but the same features will be displayed; i.e., new normal modes have to be introduced to obtain independent Schrödinger equations, and the wavefunctions are Hermite functions with slightly different scaling lengths. The calculation shows that the wavefunctions are not simply linear combinations of the wavefunctions of each individual level, but that all other states are coming in. This is not surprising since, contrary to the usual perturbation procedure which is cut off after a certain order, the solutions are exact.

The second part of the considerations, i.e., what happens if we excite one of the oscillators could only be followed experimentally if it were possible to decouple the modes temporarily.

2. THE EXACT SOLUTION

The Hamiltonian of a set of two identical coupled oscillators in one dimension is

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x_1^2}+\frac{\partial^2\psi}{\partial x_2^2}\right) + (\tfrac{1}{2}kx_1^2+\tfrac{1}{2}kx_2^2+\kappa x_1x_2)\psi = E\psi, \quad (2.1)$$

where κ is the coupling constant. The same transformation in configuration space as is used in the classical case will bring the potential energy in diagonal form. (The fact that we use two identical harmonic oscillators was just for convenience since this step can be taken just as well in the general case, as holds for most of the arguments below.)

$$y_1 = (x_1+x_2)/\sqrt{2}, \quad (2.2a)$$

$$y_2 = (x_1-x_2)/\sqrt{2}. \quad (2.2b)$$

The ∇^2 operator is invariant under a unitary (actual orthogonal) transformation and, hence the new Hamiltonian operator is

$$\mathcal{H} = -\frac{\hbar^2}{2m}(\nabla_{y_1}^2+\nabla_{y_2}^2)+\tfrac{1}{2}k_1y_1^2+\tfrac{1}{2}k_2y_2^2, \quad (2.3)$$

where $k_1=k+\kappa$, and $k_2=k-\kappa$. The resulting differential equation is separable, and the general solution is the following linear combination of all different product solutions of the individual equations.

$$\psi = \sum C_{n_1n_2}\varphi_{n_1}\varphi_{n_2}, \quad (2.4)$$

$$\varphi_{n_1} = N_{n_1}H_{n_1}(\xi_1)\exp[-\tfrac{1}{2}\xi_1^2-iE_{n_1}t/\hbar], \quad (2.5a)$$

$$\varphi_{n_2} = N_{n_2}H_{n_2}(\xi_2)\exp[-\tfrac{1}{2}\xi_2^2-iE_{n_2}t/\hbar], \quad (2.5b)$$

where H is a Hermite polynomial, N its normalization constant, and ξ_1 and ξ_2 are given by

$$\xi_1 = a_1y_1 = a_1(x_1+x_2)/\sqrt{2}; \quad a_1^4 = mk_1/\hbar^2 \quad (2.6a)$$

$$\xi_2 = a_2y_2 = a_2(x_1-x_2)/\sqrt{2}; \quad a_2^4 = mk_2/\hbar^2. \quad (2.6b)$$

The relevant quantities are of course the "scale-factors" a_1 and a_2 which differ for each oscillator.

In order to anticipate the arguments for the next section we will assume that the system was at $t<0$ in such a state that $\kappa=0$ and one oscillator, say the first one, was in the ground state, and the other in the first excited state:

$$t\leqslant 0: \quad \psi = N_0N_1H_0(x_1)H_1(x_2) \times\exp[-\tfrac{1}{2}a(x_1^2+x_2^2)-iEt/\hbar], \quad (2.7)$$

where $a^4=mk/\hbar^2$ and E is given by the sum of the energies of the individual oscillators. Actually E is irrelevant since we use (2.7) only for $t=0$.

In order to obtain the coefficients in Eq. (2.4) for this special initial condition, we have to evaluate the following integral which is obtained by multiplying the left- and right-hand side of (2.4) by (2.5), and applying orthogonality.

[2] E. Fermi, Z. Physik **71**, 250 (1931). Fermi made some estimates for the binding constants. As a result of his theory the precise wavenumbers were determined experimentally. See G. Herzberg, *Infrared and Raman Spectra of Polyatomic Molecules* (D. Van Nostrand, Inc., Princeton, New Jersey, 1945), p. 217.

$$C_{nm}=\int\psi\varphi_n(1)\varphi_m(2)d\tau_1 d\tau_2$$
$$=N_0N_1N_nN_ma\sqrt{2}\left[\frac{1}{a_1a_2^2}I_n(1)J_m(2)+\frac{1}{a_1^2a_2}I_m(2)J_n(1)\right], \quad (2.8)$$

$$I_n(i)=\int H_n(y)\exp(-\tfrac{1}{2}\alpha_i^2y^2)dy, \quad (2.9a)$$

$$J_n(i)=\int yH_n(y)\exp(-\tfrac{1}{2}\alpha_i^2y^2)dy, \quad (2.9b)$$

$$\alpha_i^2=1+a^2/a_i^2. \quad (2.10)$$

If we introduce

$$\beta_i^2=(2-\alpha_i^2)/\alpha_i^2=(a_i^2-a^2)/(a_i^2+a^2),$$

we find for the product

$$I_n(i)J_m(j)=\frac{2\pi}{\alpha_i\alpha_j}\beta_i^n(\tfrac{1}{2}\beta_j^{m+1}+m\beta_j^{m-1}) \quad (2.11)$$

if $n=$even and $m=$odd; otherwise, the product is zero. Hence if n and m have different parity either one or the other term in (2.8) is nonzero, and if n and m have the same parity the coefficient C_{nm} will be zero.

Substituting this in (2.4) will give the time-dependent wavefunction. Its explicit form is

$$\psi(\xi_1\xi_2,t)=\sum_{nm}C_{nm}N_nH_n(\xi_1)N_mH_m(\xi_2)\exp\left[\frac{it}{\hbar}\{(n+\tfrac{1}{2})\hbar\omega_1+(m+\tfrac{1}{2})\hbar\omega_2\}\right], \quad (2.12)$$

where C_{nm} is given by (2.8) and (2.11) and $\omega_i^2=k_i/m$; $(i=1, 2)$.

The time-dependent perturbation method is, so to speak, an attempt to write the expression (2.12) in a form in which the exponential contains ω, instead of ω_1 and ω_2. This is, of course, impossible, and hence the constants C are modified into time-dependent coefficients.

3. TIME-INDEPENDENT SOLUTION

In order to obtain the first-order time-independent solution we have to consider first the degeneracy of the problem. As long as the two equivalent oscillators are independent their energy states are counted individually and hence are nondegenerate since we consider linear oscillators. If we consider the two oscillators as one system, as in statistical mechanics, the degeneracy is $n+1$. This is the number of ways in which the integer n can be divided in two parts n_1 and n_2, including zero.

When we consider the secular matrix we find nonzero matrix elements only if the conditions $n_1'=n_1\pm1$ and $n_2'=n_2\mp1$ are simultaneously fulfilled. If we order the elements in an appropriate manner (increasing n_1 and decreasing n_2) we have two sets of elements parallel to the main diagonal reminiscent of the matrix of the L_x operator. The shape of the matrix is not the only thing they have in common: they are identical provided we take $j=n/2$ and $m=\frac{1}{2}(n_1-n_2)$. Hence the matrix can be diagonalized by a transformation in function space using the so-called D coefficients[3] corresponding, for instance, to a rotation $\pi/2$ around the y axis which brings the x axis into a z axis. The eigenvalues are proportional to m, hence to $\frac{1}{2}(n_1-n_2)$.

This corresponds to the second term in the power series development of the correct coupled energy levels in terms of the coupling constant

$$E=(n_1+\tfrac{1}{2})\hbar\left(\frac{k+\kappa}{m}\right)^{\frac{1}{2}}+(n_2+\tfrac{1}{2})\hbar\left(\frac{k-\kappa}{m}\right)^{\frac{1}{2}}$$
$$=(n+1)\hbar\omega+\tfrac{1}{2}(n_1-n_2)\hbar\omega\frac{\kappa}{k}-\tfrac{1}{8}(n_1+n_2+1)\hbar\omega\left(\frac{\kappa}{k}\right)^2+\cdots. \quad (3.1)$$

In order to obtain the third term in this expansion by means of time-independent perturbation we would have to transform the $n+1$ wavefunctions in the manner indicated above. It is possible and actually preferable to avoid this. In the representation corresponding to L_x, the matrix elements connecting a state having a certain n_1 and n_2 of the level $E_n(n=n_1+n_2)$ with the wavefunctions of $E_{n\pm2}$ are extremely simple, and the performance of the diagonalization of the secular matrix would destroy this simplicity.

If we calculate the matrix elements between E_n and $E_{n\pm2}$ we are dealing with a system in

[3] E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959).

which both initial and final levels are degenerate. Suppose we wanted to determine the proper linear combinations in each set; let the label be ν for the set connected with E_n and μ for the intermediate set belonging to $E_{n'}$ $(n'=n\pm 2)$.

The second-order perturbation is

$$E_{n,\nu}=\sum_{\mu}\frac{|\langle\nu|H'|\mu\rangle|^2}{E_n-E_{n'}}. \tag{3.2}$$

Since $E_{n'}$ is independent of μ the expression corresponds to a simple contraction and the choice for the linear combinations is arbitrary. Hence we prefer to use the original set labeled by n_1' (or $n'=n_1'+n_2'$):

$$\langle\nu|H'|\mu\rangle\langle\mu|H'|\nu\rangle=\langle\nu|H'|n_1'\rangle\langle n_1'|H'|\nu\rangle.$$

The same argument can be used for the initial level if we sum over ν, and divide through by $n+1$, since E_n is independent of ν at least in second order.

$$E_n^{(2)}=\frac{1}{n+1}(E_n-E_{n'})^{-1}\sum_{\nu\mu}|\langle\nu|H'|\mu\rangle|^2$$

$$=\frac{1}{n+1}(E_n-E_{n'})^{-1}\sum_{n_1n_1'}|\langle n_1|H'|n_1'\rangle|^2. \tag{3.3}$$

The last argument can be calculated directly from the well-known selection rules for the harmonic oscillator. For the transition $n\rightarrow n+2$ we have

$$|\langle\ \rangle|^2=\tfrac{1}{4}(\hbar\omega)^2\sum_{n_1=0}^{n}(n_1+1)(n-n_1+1) \tag{3.4a}$$

and for the transition $n\rightarrow n-2$ we have

$$|\langle\ \rangle|^2=\tfrac{1}{4}(\hbar\omega)^2\sum_{n_1=1}^{n-1}n_1(n-n_1). \tag{3.4b}$$

After multiplication with the energy denominators $(\pm 2\hbar\omega)^{-1}$ we find for the total contribution to this matrix element:

$$E_n^{(2)}=\tfrac{1}{8}(n+1)\hbar\omega$$

in accordance with the previous result.

4. THE TIME-DEPENDENT PERTURBATION THEORY

The ordinary time-dependent transition probability theory as found in the standard text books[4] consists of two parts. The first part is a variation of constants technique in Heisenberg representation where the resulting differential equations are solved by an iteration technique.

Usually not more than the first step is really calculated. The second part is to translate this time-dependence of the amplitude into a rate of decay of a certain state. The last part is only applicable to a system with continuous energy spectrum and is not of interest here.

We first show that the method can be slightly modified to give the correct dependence for a longer time interval. If we call the unperturbed wavefunction φ_k, and the correct eigensolution of the perturbed problem ψ_k we have for $t<0$

$$\Psi=\sum a_k e^{i\omega_k^0 t}\varphi_k \tag{4.1a}$$

and for $t>0$

$$\Psi=\sum b_k e^{i\omega_k t}\psi_k \tag{4.1b}$$

$\hbar\omega_k^0=E_k^0$ the unperturbed energy. At $t=0$ these functions should be identical

$$\sum a_k\varphi_k=\sum b_k\Psi_k. \tag{4.1}$$

Suppose $a_l=1$ and all other zero, we have

$$\varphi_l=\textstyle\sum_k\psi_k b_k. \tag{4.2}$$

Hence, if we introduce the expansion of the perturbed eigenfunctions into the unperturbed eigenfunctions

$$\psi_k=\textstyle\sum_j\varphi_j S_{jk} \tag{4.3}$$

then the amplitudes b_k are given by

$$b_k=S_{lk}^* \tag{4.4}$$

the result for $t>0$ is

$$\Psi(t)=\textstyle\sum_k S_{lk}^* e^{i\omega_k t}\psi_k$$
$$=\textstyle\sum_k S_{lk}^* e^{i\omega_k t}\sum_j\varphi_j S_{jk}. \tag{4.5}$$

If we substitute the result from the time-independent perturbation theory then,

$$S_{km}=\delta_{km}+[H_{km}'/(E_m-E_k)]+\cdots. \tag{4.6}$$

We introduce a coefficient $C_j(t)$ that would stay equal to the following constants

$$C_l=1;\quad C_j=0\quad (j\neq l) \tag{4.7}$$

if the perturbation were not switched on at $t=0$. The state vector is

$$\Psi(t)=\textstyle\sum_j C_j(t)\varphi_j \tag{4.8}$$

[4] See, for instance, L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955).

and the coefficient C_j $(j\neq l)$ given by

$$C_j(t)=\sum_k\left[\delta_{kl}+\frac{H_{lk}^{*\prime}}{E_k-E_l}\cdots\right]\times e^{i(\omega_k-\omega_l)t}\left[\delta_{kj}+\frac{H_{jk}}{E_k-E_j}\cdots\right]=\frac{H_{jl}'}{E_l-E_j}[1-e^{i(\omega_j-\omega_l)t}]+\cdots. \quad (4.9)$$

This result is almost the same as that obtained by the variation of constants technique followed by the iterative solution except that the frequency is ω instead of ω^0. This difference is important in case we have degeneracy, since the levels will be split under the influence of the perturbation, and each component has a slightly different frequency.

We will now describe the modification for the case in which the initial level is degenerate and only one of the components is "excited." In this case we have one oscillator in state n_1, the other in the ground state. All other components of the degenerate level are those values n_1' and n_2' that add up to the same total n value. The wavefunctions belonging to the degenerate level, after the perturbation is switched on, will have normal modes, whose amplitudes we indicate by β_k. The time dependent behavior is given by

$$\alpha_i(t)=\sum_k S_{ik}\beta_k e^{i\Delta\omega_k t}, \quad (4.10)$$

and the β's are determined by the initial condition

$$\alpha_\nu=1;\quad \alpha_i=0\quad (i\neq\nu)$$

where ν refers to the initially "excited" level. For

$$\beta_k=S_{\nu k}^*, \quad (4.11)$$

$$\alpha_i(t)=\sum_k S_{ik}S_{\nu k}^* e^{i\Delta\omega_k t}. \quad (4.12)$$

Both sides of Eqs. (4.10) and (4.12) are divided by $\exp i\omega^0 t$, where ω^0 is the energy of the levels before the perturbation was switched on. The occupation of the levels is given by

$$|a_i|^2=(\sum_k S_{ik}S_{\nu k}^* e^{i\Delta\omega_k t})\times(\sum_l S_{il}^* S_{\nu l} e^{-i\Delta\omega_k t}). \quad (4.13)$$

Subtracting the identity

$$|\sum S_{ik}S_{\nu k}^*|^2=\delta_{i\nu} \quad (4.14)$$

$$|a_i|^2=\delta_{i\nu}+\sum_{k<l} S_{ik}S_{\nu k}^* S_{il}^* S_{\nu l}(e^{i(\Delta\omega_k-\Delta\omega_l)t}-1)+\text{c.c.}=\delta_{i\nu}+\sum_{k<l}\mathrm{Im}(S_{ik}S_{\nu k}^* S_{il}^* S_{\nu l})\times 2i\sin(\Delta\omega_k-\Delta\omega_l)t-\sum_{k<l}\mathrm{Re}(S_{ik}S_{\nu k}^* S_{il}^* S_{\nu l})\times 4\sin^2\tfrac{1}{2}(\Delta\omega_k-\Delta\omega_l)t. \quad (4.15)$$

In the absence of a magnetic field the unitary transformation that diagonalizes the secular determinant can be chosen real. Hence,

$$|a_i|^2=\delta_{i\nu}-\sum_{k<l} 4S_{ik}S_{\nu k}S_{il}S_{\nu l}\times\sin^2\tfrac{1}{2}(\Delta\omega_k-\Delta\omega_l)t. \quad (4.16)$$

If we take the simple case in which $n_1=1$ and $n_2=0$ we have twofold degeneracy. The product of the four S factors is $\frac{1}{4}$ for $i=\nu$ and $-\frac{1}{4}$ for $i\neq\nu$ and the state a_i is depleted and occupied with a frequency $\Delta\omega_1-\Delta\omega_2$ which is proportional to the coupling constant.

APPENDIX

With the help of the usual generating function method we find

$$\sum_{n=0}\frac{s^n I_n(i)}{n!}=\int\exp(-s^2+2sy-\tfrac{1}{2}\alpha^2y^2)dy=\frac{(2\pi)^{\frac{1}{2}}}{\alpha}\exp[s^2(2-\alpha^2)/\alpha^2]=\frac{(2\pi)^{\frac{1}{2}}}{\alpha}\sum_{m=0}^{\infty}\frac{1}{m!}\left(\frac{2-\alpha^2}{\alpha^2}\right)^m s^{2m}. \quad (A1)$$

Hence,

$$I_n=[(2-\alpha^2)/\alpha^2]^{n/2}[(2\pi)^{\frac{1}{2}}/\alpha] \quad (A2)$$

for n is even and zero for $n=$ odd for every value of α, except $\alpha^2=2$. In this case:

$$I_n=\delta_{n0}[(2\pi)^{\frac{1}{2}}/\alpha]. \quad (A3)$$

The second integral can be obtained from the first using

$$yH_n=\tfrac{1}{2}H_{n+1}+nH_{n-1} \quad (A4)$$

giving

$$J_n=\frac{(2\pi)^{\frac{1}{2}}}{\alpha}\left[\frac{1}{2}\left(\frac{2-\alpha^2}{\alpha^2}\right)^{(n+1)/2}+n\left(\frac{2-\alpha^2}{\alpha^2}\right)^{(n-1)/2}\right]. \quad (A5)$$