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Note

On the bifurcation analysis of a three-dimensional non-autonomous model of molecular systems

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Bifurcations and stability of a molecular system are analyzed via a method which combines a perturbation skim with Harmonic Balancing.

Nonlinear dynamics of atomic and molecular systems have been receiving considerable attention. Miniaturization of electronic devices and the behaviour of fast computers, for example, requires a careful study of dynamics at atomic and molecular levels. It is observed that bifurcation and stability theories can play a very significant role in understanding and predicting the behaviour of such systems. The underlying dynamics, however, is quite complex and requires a non-linear analysis. A number of mathematical models has been produced for this purpose.

A three-dimensional "semi-classical" model was originally developed [3,4] for the investigation of infra-red (IR) multi-photon excitation of poly-atomic molecules. This model involves a simplified quantum formulation which yields three autonomous equations. A detailed *analytical* treatment of this model, including static and dynamic bifurcations (Hopf bifurcation) and post bifurcation behaviour, has recently been presented [5]. In that paper, the Intrinsic Harmonic Balancing (IHB) technique [2] has been applied to the autonomous set of equations to obtain quantitative analytical results concerning the cusp catastrophe as well as Hopf bifurcations and the stability of both the equilibrium states and the limit cycles exhibited by the model.

As an extension of these studies, a *non-autonomous* model is now introduced which consists of the following equations:

$$\begin{aligned}
\dot{z}_1 &= -z_1 + \phi z_2 - \alpha z_2 z_3 \equiv Z_1(z_i, \eta, \phi; \Omega t),\\
\dot{z}_2 &= -\phi z_1 - z_2 + \alpha z_1 z_3 - (\eta + E\cos\Omega t) \equiv Z_2(z_i, \eta, \phi; \Omega t),\\
\dot{z}_3 &= -2(\eta + E\cos\Omega t) z_2 - \lambda z_3 \equiv Z_3(z_i, \eta, \phi; \Omega t),
\end{aligned} \tag{1}$$

where the z_i ($i = 1, 2, 3$) are the state variables, z_1, z_2 denote the average values of the coordinate and momentum proportional to real and imaginary parts of $\langle a \rangle$, z_3 denotes $\langle a^+ a \rangle$, the operators a^+, a are the usual harmonic-oscillator type ladder operators,

ϕ and η are two independent parameters which are known as detuning parameter and Rabi rate, respectively, and α and λ are treated as constants. E and Ω are the amplitude and frequency of the harmonic excitation, respectively. Setting $E = 0$ yields the corresponding autonomous system studied earlier [5].

This model is expected to exhibit more complex phenomena, compared to the autonomous system, and the effect of harmonic excitation on the behaviour of the system is a point of interest. Indeed, it can be shown that quasi-periodic motions (on a torus) bifurcate from a periodic motion, and as a result of the harmonic excitation, the critical value of a parameter (Hopf bifurcation point) shifts to another value.

In order to analyse the behaviour of system (1), a non-singular transformation of the form $z = Aw$ ($|A| \neq 0$) is introduced such that the resulting system

$$\dot{w}_i = W_i(w_j, \mu; \Omega t) \tag{2}$$

is referred to a (critical) Hopf bifurcation point of $E = 0$ system, where $\mu = \eta - \eta_c$ and $\phi = \phi_c$, and the Jacobian of (2) at this point is in a canonical form with a pair of imaginary eigenvalue and a real eigenvalue. Scaling the variables as

$$w_i \rightarrow \varepsilon w_i, \quad \mu \rightarrow \varepsilon\mu \quad \text{and} \quad E = \varepsilon E$$

and assuming that internal and external frequencies satisfy the non-resonance condition that they are not rationally linked, one can assume both the periodic and quasi-periodic solutions to be in the parametric form

$$\begin{aligned} w_i &= w_i(\tau_1, \tau_2; \varepsilon), \\ \mu &= \mu(\varepsilon), \end{aligned} \tag{3}$$

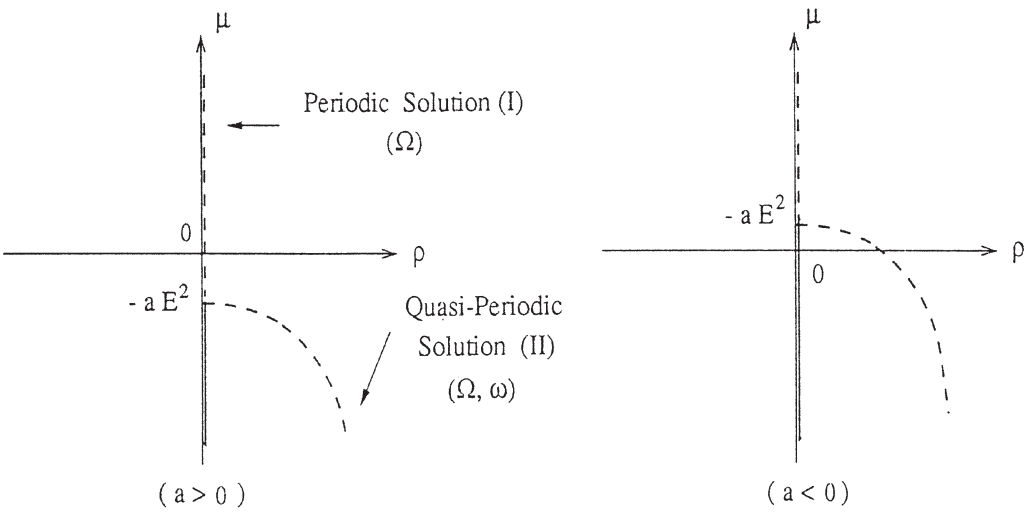

Figure 1. Bifurcation Diagram. Ω: the excitation frequency. a: is a function of (Ω); i.e., for a given Ω, a is a constant. E: is the amplitude of the excitation. ρ: is a measure of amplitude characterizing the solutions. μ: is a parameter representing the Rabi rate. ω: is a frequency associated with solutions.

where $\tau_1 = \Omega t$ and $\tau_2 = \omega(\varepsilon)t$, and $\omega(\varepsilon)$ is the frequency of the periodic solutions. One can now apply the Intrinsic Harmonic Balancing technique [2] with the aid of a two-time scale Fourier series

$$w_i(\tau_1, \tau_2; \varepsilon) = \sum_{m=0}^{M} p_{im_1m_2}(\varepsilon)\cos(m_1\tau_1 + m_2\tau_2) + r_{im_1m_2}(\varepsilon)\sin(m_1\tau_1 + m_2\tau_2), \quad (4)$$

where $m = m_1 + m_2$, m, m_1 and m_2 are integers and $m \geqslant 0$ while m_1 and m_2 may be chosen as positive or negative, and M is an arbitrary positive integer. It is noted that (4) reduces to ordinary Fourier series in the case $m_1 \equiv 0$ or $m_2 \equiv 0$. The former case ($m_1 \equiv 0$) describes periodic solutions of the associated autonomous system considered in [5] while the latter case ($m_2 \equiv 0$) denotes periodic solutions which are purely excited by the external force $E\cos\Omega t$. ε is used as a small positive perturbation parameter, and perturbation steps are carried out with the aid of MAPLE, a symbolic computer language [1].

This perturbation technique yields the information for constructing the solutions in the form of a Taylor series, asymptotically:

$$\begin{aligned} w_i(\tau_1, \tau_2; \varepsilon) &= w_i^o(\tau_1, \tau_2) + w_i'(\tau_1, \tau_2)\varepsilon + \tfrac{1}{2}w_i''(\tau_1, \tau_2)\varepsilon^2 + \cdots, \\ \mu(\varepsilon) &= \mu^o + \mu'\varepsilon + \tfrac{1}{2}\mu''\varepsilon^2 + \cdots, \\ \omega(\varepsilon) &= \omega_c + \omega'\varepsilon + \tfrac{1}{2}\omega''\varepsilon^2 + \cdots. \end{aligned}$$

The stability of solutions can also be examined. The results show that $\mu = -\mathrm{a}E^2$ (where a depends on Ω) represents a critical relation, at which quasi-periodic motions bifurcate from the periodic motions as depicted in figure 1, and an exchange of stabilities occur. Here ρ is a measure of amplitude, and full (dashed) lines indicate stable (unstable) paths. It is observed that the critical value of μ shifts from $\mu = 0$ (for the corresponding autonomous system) to $\mu = -\mathrm{a}E^2$; this is the effect of the harmonic excitation introduced to the model.

The details of this analysis as well as the effect of resonance will be presented in two full-length papers in due course.

References

[1] B.W. Char, K.O. Geddes, G.H. Gonnet, B.L. Leong, M.B. Monagan and S.M. Watt, *Maple V* (Springer-Verlag, Berlin, 1991).

[2] K. Huseyin, *Multiple Parameter Stability Theory and its Applications: Bifurcations, Catastrophes, Instabilities*, Oxford Engineering Science Series 18 (Oxford University Press, Oxford, 1986).

[3] L.M. Narducci, S.S. Mitra, R.A. Shatas and C.A. Coulter, Physics Review A 16 (1977) 247.

[4] L.M. Narducci and J.M. Yuan, Physics Review A 22 (1980) 261.

[5] U. Taneri, K. Huseyin and P. Yu, Dynamics and Stability of Systems 110 (2) (1995) 149.