Chapter 1

Classical dynamics of magnetically coupled spins

Benjamin Skellett
School of Information Technology and Electrical Engineering
The University of Queensland
ben@itee.uq.edu.au
Catherine A Holmes
Department of Mathematics
The University of Queensland
cah@maths.uq.edu.au

We investigate the dynamics of a nonintegrable system comprising of two coupled spins. This Hamiltonian system can be considered as a model for two magnetic molecules coupled via a particular nonlinear interaction. A model like this has been proposed as a realisation for quantum bits in quantum computing. We identify a critical value of the coupling parameter. Below this critical value, motion is approximately regular and the system is robust to weak coupling. Above the critical value the system bifurcates and motion can be localised about the additional elliptic fixed points. The localised motion is typically regular, though for less extreme energy values an extensive chaotic region leads to unpredictable behaviour. The energy of the system plays a crucial role in determining the accessible regions of phase space and the behaviour of the system.

1.1 Introduction

Chaos in Hamiltonian systems is remarkable because chaotic regions can be densely interweaved with regular regions in an extremely complicated phase space which is neither totally regular or ergodic. Unlike the strange attractors

of dissipative systems, there are no attractive regions in the phase space of Hamiltonian systems. As such chaos tends to explore sub-regions of the phase space bounded by regular motion[4].

The dynamics of a Hamiltonian system are completely specified by the Hamiltonian: a scalar function of position and momentum which represents the total energy of the system. Trajectories move throughout phase space conserving the Hamiltonian. Establishing the restrictions arising from energy conservation is vital to understanding the system and analysing the dynamics.

Many examples of nonintegrable spin systems have been studied using Hamiltonian mechanics[2, 5, 6]. The unusual feature of the two-spin system studied in this paper is that the coupling introduces nonlinearity into the otherwise linear system. As a result of the nonlinear interaction this simple system is capable of generating a wide range of complex dynamical behaviour.

Coupled spin systems of this kind are of much interest to quantum computing.

1.2 Physical motivation

Recently, magnetic molecules have been suggested as a realisation for quantum bits[7]. Magnetic molecules are nanometre scale molecular clusters that consist of thousands of electrons and nucleons, that can be treated as mesoscopic particles having properties such as magnetic moment and angular momentum. It is of fundamental importance to quantum computing that these magnetic qubits interact with one another in order to generate entanglement between the states[1]. Entanglement is correlation of a special kind. If two systems do not interact, they cannot be correlated.

In the system in question the interaction is achieved by coupling the magnetic clusters via superconducting loops such that the supercurrent induced in the loop by one spin produces a magnetic field at the site of the other. An external magnetic field in the z direction also acts on each molecule causing the magnetic moment, and with it the angular momentum, to *precess uniformly* about the axis parallel to the magnetic field. This is known as Larmor precession[3]. The Hamiltonian for each individual cluster[1] is simply $H_i = \omega_i L_{z_i}$, where ω_i is the Larmor frequency for each spin, determined by the external magnetic field and the mass and charge of the molecule.

In the present model, the interaction causes rotation about the y axis for each cluster with frequency proportional to the y component of the magnetic moment of the *other* cluster. Since the magnetic moment is parallel to the angular momentum, the interaction Hamiltonian can be written in terms of the y components of angular momentum, L_{y_i}, with χ being the coupling parameter:

$$H_{\text{int}} = \chi L_{y_1} L_{y_2}. \tag{1.1}$$

[1] Throughout this study the subscripts i and j are used to denote the two spins. The convention used is that $i, j \in \{1, 2\},\ i \neq j$.

The Hamiltonian of the coupled two-spin system is

$$H = \omega_1 L_{z_1} + \omega_2 L_{z_2} + \chi L_{y_1} L_{y_2}. \tag{1.2}$$

In addition to H remaining constant, the *total* angular momentum of each cluster is conserved so that $|\mathbf{L}_1|$ and $|\mathbf{L}_2|$ are also constants of the motion. By setting $|\mathbf{L}_1| = |\mathbf{L}_2| = L$ the six dimensional angular momentum phase space is constrained to the four dimensional surface of two spheres with radius, L, such that

$$\mathbf{L}_i \cdot \mathbf{L}_i = {L_{x_i}}^2 + {L_{y_i}}^2 + {L_{z_i}}^2 = L^2. \tag{1.3}$$

A point on sphere i represents the position of the axis of rotation of molecule i and the state of the system can be specified by four coordinates. The two spins form a time-independent Hamiltonian system with two degrees of freedom.

1.3 Analysis

Using the Poisson bracket and its angular momentum relations[3], the equations of motion for each spin can be determined:

$$\dot{L_{x_i}} = -\omega_i L_{y_i} + \chi L_{z_i} L_{y_j}, \tag{1.4}$$

$$\dot{L_{y_i}} = \omega_i L_{x_i}, \tag{1.5}$$

$$\dot{L_{z_i}} = -\chi L_{x_i} L_{y_j}. \tag{1.6}$$

When $\chi = 0$, L_{z_i} is constant and (L_{x_i}, L_{y_i}) rotate about the z axis with frequency, ω_i. Alternatively, if $\omega_1 = \omega_2 = 0$, L_{y_i} is constant and (L_{x_i}, L_{z_i}) rotate about the y axis with frequency χL_{y_j}, $(i \neq j)$. More complex dynamics occur when both of these influences affect the motion.

Figure 1.1 shows a sample of the behaviour that the spins can exhibit for different parameters. One spin is shown for each regime. The variety of possible dynamics of the system necessitates an analytic approach to investigate and categorize the behaviour.

One way to represent the four dimensional phase space is to use a stereographic projection and map each sphere $(L_{x_i}, L_{y_i}, L_{z_i})$ onto a plane (α_i, β_i) such that the 'north pole' $(L_{z_i} = L)$ is mapped to the origin, the 'south pole' $(L_{z_i} = -L)$ is mapped to infinity, and the 'equator' $(L_{z_i} = 0)$ is mapped to the unit circle, ${\alpha_i}^2 + {\beta_i}^2 = 1$. This is not an area preserving transformation, however it does preserve angles and the resulting phase space is only four dimensional.

The phase flow in the $(\alpha_1, \beta_1, \alpha_2, \beta_2)$ coordinates is described by:

$$\dot{\alpha_i} = -\omega_i \beta_i + \chi L \beta_j \frac{(1 + {\alpha_i}^2 - {\beta_i}^2)}{(1 + {\alpha_j}^2 + {\beta_j}^2)}, \tag{1.7}$$

$$\dot{\beta_i} = \omega_i \alpha_i + 2\chi L \frac{\alpha_i \beta_i \beta_j}{(1 + {\alpha_j}^2 + {\beta_j}^2}. \tag{1.8}$$

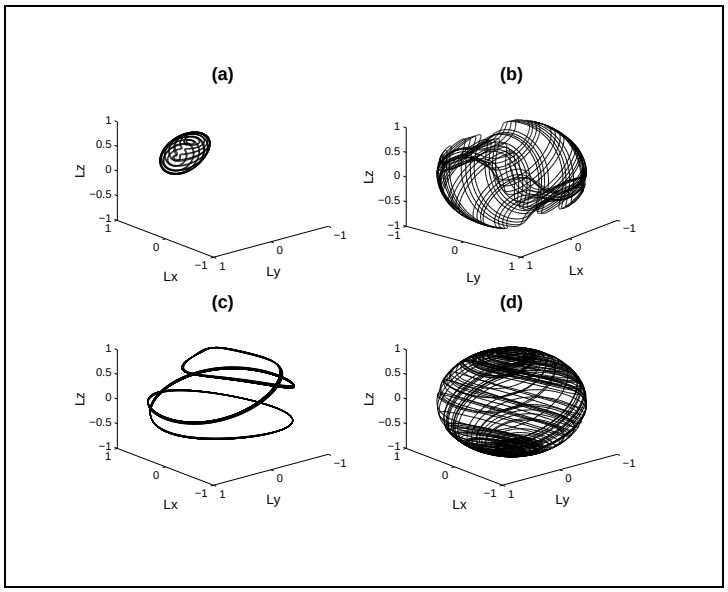

Figure 1.1: (a) Localised regular motion. (b) Regular motion exploring more of the phase space. (c) Densely clustered trajectories. (d) Globally chaotic motion.

As with equations 1.4, 1.5, 1.6, the dynamics of the uncoupled system ($\chi = 0$) are simple in this new representation however the nonlinearity is quite complex. This is further complicated by the fact that motion near the south pole requires α and β to approach infinity. As such motion near the south pole can be distorted by this projection.

Fixed points in angular momentum space represent equilibrium solutions where the angular momentum of both spins remains constant. The origin ($\uparrow\uparrow$) is a fixed point and there exist four more fixed points when χ exceeds the threshold value:

$$\chi_{\mathrm{c}} = \frac{\sqrt{\omega_1 \omega_2}}{L}. \tag{1.9}$$

The south pole configuration ($\downarrow\downarrow$) is also a fixed point of the system. Further analysis shows that at $\chi = \chi_{\mathrm{c}}$ a supercritical pitchfork bifurcation occurs destabilising the existing fixed points. As χ increases, two elliptic fixed points emerge in opposite directions from each pole along the L_{y_i} (or β_i) axis. For large χ these points aymptotically approach the equator meaning there are always two elliptic fixed points in each hemisphere.

The total energy of the system (equation 1.2) is determined by the starting momenta of the spins. For χ subcritical, the angular momentum constraint (equation 1.3) results in the energy being maximum when both spins are at the north pole and minimum when both spins are at the south pole. These extreme energy values are $H = \pm(\omega_1 + \omega_2)L$. When χ is above the threshold value,

extreme energy values occur when $\nabla H = 0$. With χ supercritical, the energy is maximum at the stable fixed points in the northern hemisphere and is minimum at the stable fixed points in the southern hemisphere.

Trajectories can only travel in regions of phase space that have the same energy thus it makes intuitive sense that the stable fixed points have extreme energy values, confining motion to the fixed point. Motion near a stable fixed point is confined to a sub-region of the phase space that has a constant energy close to that of the extreme value. Regions with the same energy define the *energy surface*: a three dimensional hypersurface on which the Hamiltonian is constant. The parameters, ω_1, ω_2 and χ, and the starting momenta determine the topology of the energy surface which is fundamental in establishing the accessible regions of phase space.

This surface can be visualised by considering its two dimensional intersection with the hypersurface $\alpha_1 = 0$. When $\chi = 0$ the energy surface is radially symmetric in the orthogonal coordinate system $(\beta_1, \alpha_2, \beta_2)$. As χ increases, the surface becomes warped and skewed in opposing directions until, when χ is supercritical, it is possible for the energy surface to exist as two disjoint surfaces localised around the fixed points (Figure 1.2). For negative values of energy, the energy surface appears as two infinitely wide disjoint sheets which can also extend to infinity in a tube-like manner along the perpendicular axis (Figure 1.3). This is an artifact of the stereographic projection and can be overcome by applying a different stereographic transformation.

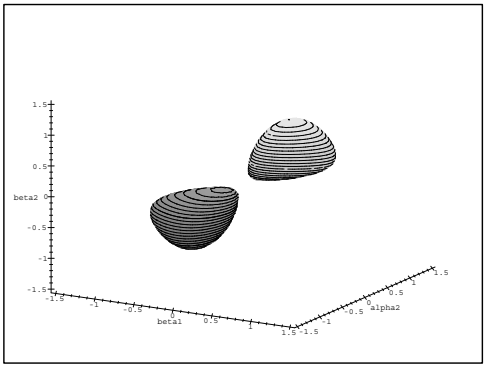

Figure 1.2: Disjoint energy surface with $H > (\omega_1 + \omega_2)L$ and $\chi > \chi_c$.

Conditions on the topology of the energy surface an be found by analysising the Hamiltonian. $H_{\uparrow\uparrow}$ is the energy of the system 'at the origin' where both spins start in the upright position:

$$H_{\uparrow\uparrow} = (\omega_1 + \omega_2)L \tag{1.10}$$

Essentially, $H_{\uparrow\uparrow}$ is an energy threshold. If $H > (\omega_1 + \omega_2)L$ the energy surface is disjoint and motion is localised around the maximum energy fixed points. Similarly, if $H < -(\omega_1 + \omega_2)L$ motion will be localised around the minimum energy fixed points.

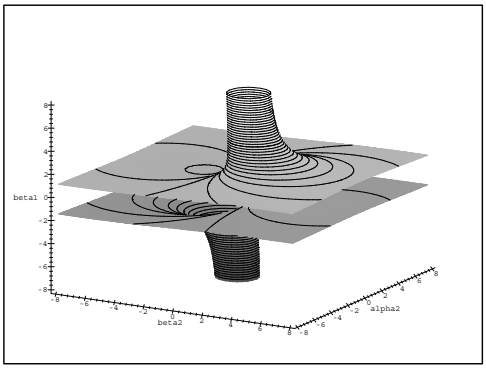

Figure 1.3: 'Infinite' energy surface with $H < 0$.

It is well established for autonomous Hamiltonian systems with two degrees of freedom that the existence of two constants of motion results in integrable dynamics[3, 4]. Integrable trajectories are constrained to the two dimensional surface of intersection described by the global invariants. The Hamiltonian is one such global invariant though it is generally difficult to determine whether another constant of the motion exists. Poincaré maps can be used to investigate whether an additional constant exists and whether the system is in fact integrable.

The Poincaré map is a numerical technique with the ability to reveal structure in seemingly disordered motion and provide a useful indication of integrable motion. It allows us to sample the motion by taking a cross section of the phase space while retaining all the information of the original phase flow. Poincaré maps for this system were generated via numerical integration of trajectories in the four dimensional phase space. The dynamics are constrained to the energy surface. When a trajectory crosses the hypersurface $\alpha_1 = 0$ in the same direction, the point of intersection is recorded in the Poincaré map. The Poincaré map reveals integrable periodic motion as closed one dimensional curves and chaos as a scatter of points, typically bounded by integrable motion.

Figure 1.4 shows a series of Poincaré maps as χ increases. As the perturbation increases the invariant curves break up and motion becomes 'globally chaotic' when a trajectory can travel unbounded over the energy surface. Even with strong coupling, motion is typically regular about the elliptic fixed points, for energy above $H_{\uparrow\uparrow}$.

1.4 Discussion

In this study we have investigated the dynamics of a coupled two-spin system as the coupling and energy change. For weak coupling, the poles are elliptically stable and motion is approximately regular. Numerical investigation displays one spin spiralling in towards the pole while the other spin spirals outwards. Governed by energy conservation, each spin's radial direction reverses and this

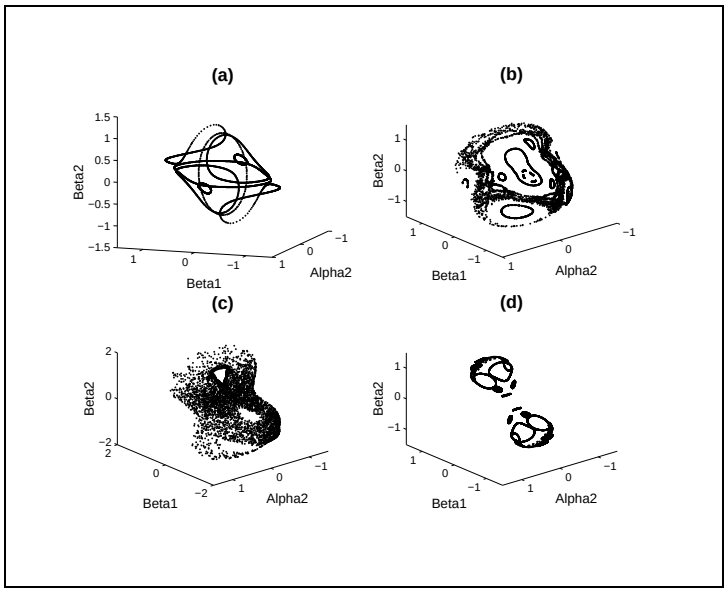

Figure 1.4: Poincaré maps for a system with $L = 1, \omega_1 = 1, \omega_2 = 1$. The critical values, $\chi_c = 1$ and $H_{\uparrow\uparrow} = 2$. (a) $\chi = 0.5, H = 1.2$. Closed curves for eight different initial conditions depicting regular, period-one behaviour. (b) $\chi = 1.2, H = 1.2$. For χ supercritical some invariant curves break up. The scatter of points displaying chaotic motion is generated from one initial condition. Period-three motion is also observed. (c) $\chi = 2, H = 1.2$. The chaotic region in this map is generated from one initial condition. It appears that some regular motion still exists and constrains the nonintegrable motion. (d) $\chi = 2, H \approx 2.07$. The energy surface is disjoint and motion is localised about the elliptic fixed points. The Poincaré map displays closed curves signifying regular behaviour for eight initial conditions on each surface. No chaotic motion is observed in this map.

cyclical motion continues indefinitely.

As χ increases, regular behaviour persists close to the origin although chaos can be observed further out for trajectories with lower energy magnitude. Chaos is caused by resonance between the two spins and is more readily observed when $\omega_1 = \omega_2$. Motion started with a lower $|H|$ also has a larger accessible energy surface which contributes to the behaviour of the system.

We have identified a critical value for the coupling parameter, χ_c at which the elliptically stable poles become hyperbolic and two elliptic fixed points emerge from each pole. This bifurcation results in qualitatively different phase space as the energy surface can become disjoint and localised around the new fixed points. Furthermore, the unstable poles no longer have extreme energy values so trajectories initially near the poles are able to traverse larger regions of phase space while maintaining constant energy.

Chaotic motion is more prevalent when χ is supercritical but is also influenced

by the energy surface. Lower $|H|$ results in an energy surface on which chaotic motion is typically more widespread. When $|H| > (\omega_1+\omega_2)L$, motion is localised around the stable fixed points and is typically regular.

Since the classical dynamics act as a guide for the quantum dynamics, the implications for quantum computing are clear. The coupled spins must behave predictably for time reversible dynamics. However, the interaction needs to allow arbitrary rotation and create measurably different states. This study suggests χ should be supercritical and $|H| > H_{\uparrow\uparrow}$ such that motion is localised about the extreme energy fixed points avoiding regions of chaos. Identifying and locating the resonances responsible for the chaotic dynamics will lead to further understanding of the complicated behaviour of this system.

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