Extraction of a Collective Submanifold for the Hénon-Heiles System

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The maximal-decoupling procedure of a collective submanifold formulated within the framework of the time-dependent Hartree-Fock theory is applied to a classical Hamiltonian system numerically investigated by Hénon and Heiles. The periodic orbits are obtained from the condition that the terms with zero denominators vanish in the collective Hamiltonian and they are in agreement with the numerical results by computer simulation.

§ 1. Introduction

The aim of this paper is to study a theory which describes a large-amplitude nuclear collective motion within the framework of the time-dependent Hartree-Fock theory (TDHF), by applying it to a simple classical system.

The TDHF equation is

\[ \delta \left\{ \langle \psi(t) | \left( i \frac{\partial}{\partial t} - H \right) | \psi(t) \rangle \right\} = 0, \] (1.1)

where \( | \psi(t) \rangle \) is a time-dependent single Slater determinant,

\[ | \psi(t) \rangle = e^{i \int_t^0 \mathcal{F}(t') dt'} | \psi_0 \rangle e^{-i \mathcal{F}_0 t}, \]

\[ \mathcal{F}(t) = \sum_{\mu} \{ f_{\mu}(t) \tilde{\alpha}_\mu \tilde{\alpha}_i + f^*_{\mu}(t) \tilde{\alpha}_i \tilde{\alpha}_\mu \}, \]

\[ \tilde{\alpha}_\mu | \psi_0 \rangle = 0, \quad \tilde{\alpha}_i | \psi_0 \rangle = 0, \quad (\mu = 1, \ldots, M; i = 1, \ldots, N) \] (1.2)

\( | \psi_0 \rangle \) being the Hartree-Fock ground state with energy \( E_0 \), and \( \tilde{\alpha}_\mu \) and \( \tilde{\alpha}_i \) denote particle-creation operators in the unoccupied single-particle orbit \( \mu \) and the occupied orbit \( i \), respectively. By an appropriate transformation from the set of variables \( \{ f_{\mu}(t), f^*_\mu(t) \} \) to a new one \( \{ C_{\mu}(t), C^*_\mu(t) \} \), the TDHF equation reduces to the classical canonical equations of motion\(^{1,2}\)

\[ i \dot{C}_{\mu} = - \frac{\partial H}{\partial C^*_\mu}, \quad i \dot{C}^*_\mu = \frac{\partial H}{\partial C_{\mu}} \] (1.3)

or

\[ \dot{q}_{\mu} = \frac{\partial H}{\partial p_{\mu}}, \quad \dot{p}_{\mu} = - \frac{\partial H}{\partial q_{\mu}}, \]

\[ q_{\mu} = \frac{1}{\sqrt{2}} (C_{\mu}^* + C_{\mu}), \quad p_{\mu} = \frac{i}{\sqrt{2}} (C_{\mu}^* - C_{\mu}) \] (1.4)

with
Further, after a linear canonical transformation, $H$ is written as

$$H = \frac{1}{2} \sum_{k=1}^{n} \omega_k (q_k'^2 + p_k'^2) + \text{(higher-order terms)},$$

ignoring rotation. Neglecting the terms of order higher than the quadratic is not always a good approximation even for low-lying excitation levels, which show anharmonicity effects. Recently, a theory which describes the large-amplitude collective motion, incorporating anharmonicity effects, has been developed.\(^1\)\(^\sim\)\(^4\) This theory gives how to extract a maximally-decoupled collective submanifold out of the TDHF manifold (or the whole phase space). To understand it better, an application to a simple system will be meaningful. We apply it to a classical Hamiltonian system first numerically investigated by Hénon and Heiles.\(^5\)\(^*)\)

In § 2, the concept of the collective submanifold is illustrated and the procedure for its extraction is given by successive canonical transformations. In § 3, the procedure is applied to the Hénon-Heiles system.

## § 2. The maximal-decoupling procedure of a collective submanifold

First, ignoring the terms of order higher than the quadratic in the Hamiltonian (1.6), we observe the following equations hold:

$$\left[ \frac{\partial H^{(2)}(q', p')}{\partial q_r'} \right] = 0, \quad \left[ \frac{\partial H^{(2)}(q', p')}{\partial p_r'} \right] = 0, \quad (r = 1, 2, \ldots, n-1)$$

(2.1)

where $H^{(i)}(q', p')$ is a sum of all the $i$th-order terms in $H(q', p')$ with respect to $q'_k$ and $p'_k$, and the symbol $[g]$ for any function $g(q', p')$ denotes its value at the point where $q_r'$ and $p_r'$ satisfy

$$q_r'(q, p) = 0, \quad p_r'(q, p) = 0 \quad \text{for any } r.$$  

(2.2)

Equation (2.1) is called a maximal-decoupling condition. It means that, if initially holds Eq. (2.2) which determines a surface called a collective submanifold, the variables $q_{\mu i}$ and $p_{\mu i}$ stay, forever, on the surface; that is, the motion is described with the variables $q_{\nu}'$ and $p_{\nu}'$ only:

$$q_{\mu i} = q_{\mu i}(q_{\nu}', p_{\nu}'), \quad p_{\mu i} = p_{\mu i}(q_{\nu}', p_{\nu}').$$

(2.3)

With the higher-order terms the same argument holds. Our task is to find a transformation to a maximal-decoupling form for $H^{(i)} (i \geq 3)$.

The present formulation is almost the same as those of Birkhoff\(^6\) and Gustavson.\(^7\) They used this method to reduce a Hamiltonian to a normal form, while

\(*\) The self-consistent collective-coordinate method (SCC), which has been developed in Refs. 2) and 3), extracts a collective submanifold by the so-called invariance principle of the (time-dependent) Schrödinger equation, while the present formulation does the same thing by imposing a maximal-decoupling condition on the classical canonical equations of motion to which the TDHF equation reduces.
we use it for the reduction to a maximal-decoupling form. Our maximal-decoupling procedure is similar to that in Ref. 4).

We assume that the excitation energy of the system is small enough to allow the power expansion in the canonical variables, and that the Hamiltonian satisfies the maximal-decoupling condition up to degree \( s-1 \):

\[
\left[ \frac{\partial H^{(i)}(P, Q)}{\partial Q_r} \right] = 0, \quad \left[ \frac{\partial H^{(i)}(P, Q)}{\partial P_r} \right] = 0. \quad (r=1, 2, \ldots, n-1; i=2, 3, \ldots, s-1)
\]  

(2.4)

Let us consider the following canonical transformation:

\[
Q_k' = Q_k + \sum_j \frac{\partial W^{(s)}(Q', P')}{\partial Q_k}, \quad P_k' = P_k + \sum_j \frac{\partial W^{(s)}(Q', P')}{\partial P_k}, \quad (k=1, 2, \ldots, n)
\]  

(2.5)

generated by a homogeneous polynomial of degree \( s \), \( W^{(s)}(Q, P') \). We have

\[
H'(Q, P', \frac{\partial W^{(s)}}{\partial Q}) = H(Q + \frac{\partial W^{(s)}}{\partial P'}, P'),
\]  

(2.6)

where \( H'(Q', P') \) is the new Hamiltonian. The general term of order \( l-j+j(s-1) \) is

\[
\frac{1}{j!} \frac{\partial^j H^{(i)}(Q, P)}{\partial P^j} \left( \frac{\partial W^{(s)}(Q', P')}{\partial Q} \right)^j \quad (j=0, 1, \ldots; l=2, 3, \ldots)
\]  

(2.7)

for the left-hand side, and

\[
\frac{1}{j!} \frac{\partial^j H^{(i)}(Q, P)}{\partial Q^j} \left( \frac{\partial W^{(s)}(Q', P')}{\partial Q} \right)^j
\]  

(2.8)

for the right-hand side with

\[
\frac{\partial^j H^{(i)}}{\partial P^j} = \sum_{j_k} \frac{\partial^j H^{(i)}}{\partial P_1^{j_1} \partial P_2^{j_2} \cdots \partial P_n^{j_n}}, \quad j = \sum_{k=1}^n j_k,
\]

\[
j! = \prod_{k=1}^n (j_k!)
\]

\[
\left( \frac{\partial W^{(s)}}{\partial Q} \right)^j = \prod_{k=1}^n \left( \frac{\partial W^{(s)}}{\partial Q_k} \right)^{j_k}
\]  

(2.9)

Picking out those terms whose degrees are equal to \( i \) yields

\[
H^{(i)}(Q, P') = H^{(i)}(Q, P') + \sum_{j \geq i} \frac{1}{j!} \left\{ \frac{\partial^j H^{(i)}}{\partial P^j} \left( \frac{\partial W^{(s)}}{\partial Q} \right)^j \right\}
\]

\[
i = l-j+j(s-1).
\]  

(2.10)

For \( i=s \), there remain only the terms with \( j=1, l=2 \):

\[
H^{(s)}(Q, P') = H^{(s)}(Q, P') + \sum_{\sigma=1}^n \omega_{\sigma} \left( P_{k} - \frac{\partial W^{(s)}}{\partial Q_k} Q_{k} \frac{\partial}{\partial P_{k}} \right) W^{(s)}(Q, P'),
\]  

(2.11)

where we use
For \( i < s \), we have
\[
H^{(i)}(Q, P') = H^{(i)}(Q, P').
\] (2·13)

Equation (2·11) can be rewritten in a more convenient form
\[
\bar{H}^{(i)}(\eta, \eta^*) = \bar{H}^{(i)}(\eta, \eta^*) + \sum_{k=1}^{s} i\omega_k \left( \eta_k \frac{\partial}{\partial \eta_k} \eta_k^* \frac{\partial}{\partial \eta_k^*} \right) \bar{W}^{(i)}(\eta, \eta^*),
\]
\[
Q_k = \frac{1}{\sqrt{2}} (\eta_k + \eta_k^*), \quad P'_k = \frac{i}{\sqrt{2}} (\eta_k - \eta_k^*),
\]
\[
\bar{H}^{(i)}(\eta, \eta^*) = H^{(i)}(Q, P'), \quad \bar{H}^{(i)}(\eta, \eta^*) = H^{(i)}(Q, P'),
\]
\[
\bar{W}^{(i)}(\eta, \eta^*) = W^{(i)}(Q, P').
\] (2·14)

By comparing the coefficient of each term, \( \bar{W}^{(i)} \) or \( W^{(i)} \) is easily determined so that the new Hamiltonian \( H'(Q', P') \) satisfies the maximal-decoupling condition up to degree \( s \); that is, it has no terms whose orders in \( Q_r' \) and \( P_r' \) (\( r = 1, 2, \ldots, n-1 \)) are equal to one up to degree \( s \). As this procedure is repeated, the transformed Hamiltonian is expected to satisfy the maximal-decoupling condition more and more accurately.

The above whole argument is straightforwardly extended to the cases where the collective motion is described by more variables.

\section*{§ 3. The application to the Hénon-Heiles system}

\subsection*{3.1. Brief review of the numerical investigation}

In 1963, Hénon and Heiles numerically investigated the Hamiltonian system
\[
H = \frac{1}{2} (q_1^2 + p_1^2 + q_2^2 + p_2^2) + q_1^2 q_2 - \frac{1}{3} q_2^3
\] (3·1)
in terms of the so-called Poincaré mapping.\textsuperscript{5} The diagrams of Fig. 1 give the successive points of intersection of various orbits in the space \((q_1, q_2, p_2)\) by the surface of section \( q_1 = 0 \) with \( p_1 = q_1 > 0 \) at the energy \( E = 1/12 \approx 0.08333 \). The passage from a point to the next one can be considered a mapping. In this mapping, a closed invariant curve, on which an infinity of points lie, represents a quasi-periodic orbit. The periodic orbits are represented by one or a finite number of invariant points. In the middle of the four small loops are four invariant points A, B, C and D, corresponding to stable periodic orbits. The three intersections of curves are also invariant points (E, F, G), corresponding to unstable periodic orbits. Further, for the energy \( E \geq 1/8 \), they discovered points scattered over a finite area, corresponding to a (semi-)ergodic orbit. This paper is concerned with the above seven periodic orbits.

\subsection*{3.2. The system of two harmonic oscillators with an equal frequency}

Before discussing the Hénon-Heiles system, we consider the system of two harmonic oscillators.
Table I. Calculated locations of the invariant points in the Poincaré mapping of the Hénon-Heiles system for \( E = 0.08333 \). The types and angles of the transformations, which they are associated with, are also shown.

<table>
<thead>
<tr>
<th>((q_n, p_n))</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
<th>G</th>
</tr>
</thead>
<tbody>
<tr>
<td>((0, -0.20))</td>
<td>I</td>
<td>I</td>
<td>II</td>
<td>II</td>
<td>I</td>
<td>I</td>
<td>I</td>
</tr>
<tr>
<td>((0, +0.20))</td>
<td>I</td>
<td>I</td>
<td>II</td>
<td>II</td>
<td>I</td>
<td>I</td>
<td>I</td>
</tr>
<tr>
<td>((0.25, 0))</td>
<td>II</td>
<td>II</td>
<td>I</td>
<td>I</td>
<td>I</td>
<td>I</td>
<td>I</td>
</tr>
<tr>
<td>((-0.31, 0))</td>
<td>(\phi = +60^\circ)</td>
<td>(\phi = -60^\circ)</td>
<td>(\phi = +45^\circ)</td>
<td>(\phi = -45^\circ)</td>
<td>(\phi = +30^\circ)</td>
<td>(\phi = -30^\circ)</td>
<td>(\phi = 90^\circ)</td>
</tr>
<tr>
<td>((0.22, -0.28))</td>
<td>(\phi = 90^\circ)</td>
<td>(\phi = 90^\circ)</td>
<td>(\phi = 90^\circ)</td>
<td>(\phi = 90^\circ)</td>
<td>(\phi = 90^\circ)</td>
<td>(\phi = 90^\circ)</td>
<td>(\phi = 90^\circ)</td>
</tr>
<tr>
<td>((0.22, +0.28))</td>
<td>(\phi = -90^\circ)</td>
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</tr>
<tr>
<td>((-0.12, 0))</td>
<td>(\phi = -90^\circ)</td>
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<td>(\phi = -90^\circ)</td>
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<td>(\phi = -90^\circ)</td>
<td>(\phi = -90^\circ)</td>
<td>(\phi = -90^\circ)</td>
</tr>
</tbody>
</table>

\[ H = \frac{1}{2}(q_1^2 + p_1^2 + q_2^2 + p_2^2), \quad (3.2) \]

neglecting the third-order terms. This Hamiltonian is invariant and remains in a maximal-decoupling form under a certain kind of linear canonical transformations, among which let us consider the following two types of transformation.

[Type I]

The first type of transformation is given by

\[
\begin{align*}
q_1' &= \begin{pmatrix} 
\cos \theta & \sin \theta 
\end{pmatrix} q_1, \\
q_2' &= \begin{pmatrix} 
-\sin \theta & \cos \theta 
\end{pmatrix} q_2, \\
p_1' &= \begin{pmatrix} 
\cos \theta & \sin \theta 
\end{pmatrix} p_1, \\
p_2' &= \begin{pmatrix} 
-\sin \theta & \cos \theta 
\end{pmatrix} p_2,
\end{align*}
\]

\[\theta = 90^\circ, \quad 0^\circ < \theta \leq 90^\circ. \quad (3.3)\]

determine a collective submanifold for each value of \(\theta\). Together with the equation of energy conservation

\[ E = \frac{1}{2}(q_1^2 + p_1^2 + q_2^2 + p_2^2), \quad (3.5) \]

they give invariant points \((q_n, p_n)\) in the Poincaré mapping for \(p_1 > 0\) when we put \(q_1 = 0\). The invariant points distribute densely on the \(p_2\) axis between \(-\sqrt{2E}\) and \(\sqrt{2E}\) (Fig. 2), corresponding to straight-line periodic orbits in the \((q_1, q_2)\) plane. The orbits are obtained by eliminating the momentum variables \(p_1\) and \(p_2\) from Eqs. (3.4) and (3.5).

[Type II]

The second type of transformation is given by

\[
\begin{align*}
q_1' &= \begin{pmatrix} 
\cos \varphi & \sin \varphi 
\end{pmatrix} q_1, \\
q_2' &= \begin{pmatrix} 
\cos \varphi & \sin \varphi 
\end{pmatrix} q_2, \\
p_1' &= \begin{pmatrix} 
-\sin \varphi & \cos \varphi 
\end{pmatrix} p_1, \\
p_2' &= \begin{pmatrix} 
-\sin \varphi & \cos \varphi 
\end{pmatrix} p_2,
\end{align*}
\]

\[\varphi < 90^\circ, \quad 0^\circ < \varphi \leq 90^\circ. \quad (3.6)\]
Fig. 2. The invariant points in the Poincaré mapping of the system of two harmonic oscillators with an equal unit frequency. The invariant points corresponding to general periodic orbits distribute in the shaded area. The invariant points corresponding to straight-line periodic orbits lie on the $p_2$ axis as shown by the thick solid line, corresponding to elliptical periodic orbits whose principal axes are the $q_1$ and $q_2$ axes and to circular orbits at $\varphi = \pm 45^\circ$.

It is easily shown that the invariant points corresponding to general periodic motions under the Hamiltonian (3.2) distribute densely in the area, $q_2^2 + p_2^2 \leq 2E$ (Fig. 2). The procedure given in §2 seems to imply that any of such periodic motions would persist even when we consider the whole Hamiltonian. However, only seven invariant points were found for $E = 1/12$ in the above-mentioned numerical experiment. At first sight this fact appears strange.

3.3. The Hénon-Heiles system

We consider the two types of linear canonical transformation taken in the preceding subsection.

[Type I]

The transformation (3.3) yields a new Hamiltonian

$$
H'(q', p') = \frac{1}{2} \left\{ \omega_1 (q_1'^2 + p_1'^2) + \omega_2 (q_2'^2 + p_2'^2) \right\} + \mu_1 q_1'^3 + \mu_2 q_2'^3 + \nu_1 q_1'^2 q_2' + \nu_2 q_1' q_2'^2
$$

(3.7)

with

$$
\begin{align*}
\omega_1 &= \omega_2 = 1, \\
\mu_1 &= (1 - \frac{4}{3} \sin^2 \theta) \sin \theta, \\
\mu_2 &= (1 - \frac{4}{3} \cos^2 \theta) \cos \theta, \\
\nu_1 &= (1 - 4 \sin^2 \theta) \cos \theta, \\
\nu_2 &= (1 - 4 \cos^2 \theta) \sin \theta,
\end{align*}

(3.8)

where the frequencies are put $\omega_1$ and $\omega_2$ to see the properties of the maximal-decoupling procedure, and are equated to unity afterwards. To obtain the Hamiltonian in a maximal-decoupling form up to degree 3,

$$
\frac{\partial H^{(i)}(q'', p'')}{\partial q_1''} = 0, \quad \frac{\partial H^{(i)}(q'', p'')}{\partial p_1''} = 0, \quad (i = 2, 3)
$$

(3.9)

we perform the canonical transformation from the set of variables $(q_k', p_k')$ to $-90^\circ < \varphi \leq 90^\circ$. After the same arguments as above, we find that the invariant points distribute densely on the $q_2$ axis between $-\sqrt{2E}$ and $\sqrt{2E}$ (Fig. 2), corresponding to elliptical periodic orbits whose principal axes are the $q_1$ and $q_2$ axes and to circular orbits at $\varphi = \pm 45^\circ$. 

After the same arguments as above, we find that the invariant points distribute densely on the $q_2$ axis between $-\sqrt{2E}$ and $\sqrt{2E}$ (Fig. 2), corresponding to elliptical periodic orbits whose principal axes are the $q_1$ and $q_2$ axes and to circular orbits at $\varphi = \pm 45^\circ$. 

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\{q^{(k)}, p^{(k)}\} (k=1, 2) generated by
\begin{align}
W^{(3)}(q', p') &= \frac{\nu_2}{4}(2aq'q''p' + bq''^2p' + cp''^2p') \\
&= \frac{\nu_2}{3}(2q'p''q' + q''^2p' + 2p''^2p'),
\end{align}
\begin{align}
a &= \frac{1}{2\omega_1 + \omega_2} + \frac{1}{2\omega_2 - \omega_1}, \\
b &= \frac{1}{2\omega_1 + \omega_2} - \frac{1}{2\omega_2 - \omega_1} + \frac{2}{\omega_1}, \\
c &= \frac{1}{2\omega_2 - \omega_1} - \frac{1}{2\omega_2 + \omega_1} + \frac{2}{\omega_1}, \tag{3.10}
\end{align}
and we have
\begin{align}
q'' &= q' + \frac{\partial W^{(3)}}{\partial p'} = q' + \frac{\nu_2}{4}(bq''^2 + cp''), \\
p'' &= p' - \frac{\partial W^{(3)}}{\partial q'} = p' - \frac{\nu_2}{2}aq'p'', \\
q'' &= q' + \frac{\partial W^{(3)}}{\partial p''} = q' + \frac{\nu_2}{2}(aq'q' + cp''p''), \\
p'' &= p' - \frac{\partial W^{(3)}}{\partial q''} = p' - \frac{\nu_2}{2}(aq''q' + bp'p''). \tag{3.11}
\end{align}
We safely carry out the same procedure up to degree 5. The generating functions $W^{(4)}$ and $W^{(5)}$ are shown in the Appendix. The obtained Hamiltonian has a form like
\begin{align}
\tilde{H}_x^{(6)}(\xi, \xi^*) &= h\xi^2\xi^3\xi^3\xi + h^*\xi^2\xi^3\xi^3\xi^* + \cdots, \\
q^{(4)} &= \frac{1}{\sqrt{2}}(\xi^h + \xi^h^*), \\
p^{(4)} &= \frac{i}{\sqrt{2}}(\xi^h - \xi^h^*), \tag{3.12}
\end{align}
where $H, q^{(i)}$ and $p^{(i)}$ denote a Hamiltonian and variables with $i$ primes, respectively. Correspondingly, the generating function which induces the transformation to a maximal-decoupling form up to degree 6 is of the form
\begin{align}
\tilde{W}^{(6)}(\xi, \xi^*) &= \frac{h}{\omega_2 - \omega_1}\xi^2\xi^3\xi^3\xi + \frac{h^*}{\omega_2 - \omega_1}\xi^2\xi^3\xi^3\xi^* + \cdots, \\
q^{(4)} &= \frac{1}{\sqrt{2}}(\xi^h + \xi^h^*), \\
p^{(4)} &= \frac{i}{\sqrt{2}}(\xi^h - \xi^h^*), \tag{3.13}
\end{align}
When we equate $\omega_1$ and $\omega_2$, it diverges* unless $h$ and $h^*$ vanish. Using the relation $3\mu_1 = -\nu_2$ and $3\mu_2 = -\nu_1$, we have

* Generally, such divergent terms can also appear in $W^{(4)}$. In the present case, they vanish for any value of $\theta$. 

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\[ h = h^* = 189 \mu_1 \mu_2 (\mu_1^2 + \mu_2^2) \]
\[ = 189 (\mu_1^2 + \mu_2^2) (1 - \frac{4}{3} \sin^2 \theta) (1 - \frac{4}{3} \cos^2 \theta) \sin \theta \cos \theta \quad (3\cdot14) \]

which vanish at
\[ \theta = 0^\circ, \pm 30^\circ, \pm 60^\circ, 90^\circ. \quad (-90^\circ < \theta \leq 90^\circ) \quad (3\cdot15) \]

The following calculation will show that each of the above values, except \( \theta = 0^\circ \), corresponds to an invariant point in Fig. 1. The invariant points A, B, E, F and G correspond to \( \theta = +60^\circ, -60^\circ, +30^\circ, -30^\circ \) and \( 90^\circ \), respectively.

For \( \theta = 0^\circ \) and \( \pm 60^\circ \), the linearly transformed Hamiltonian \( H'(q', p') \) exactly satisfies the maximal-decoupling condition
\[ \left[ \frac{\partial H'(q', p')}{\partial q'} \right] = 0, \quad \left[ \frac{\partial H'(q', p')}{\partial p'} \right] = 0, \quad (3\cdot16) \]

since \( \nu_2(-3\mu_1) \) vanishes there. In the case \( \theta = 0^\circ \), as is seen from
\[ q'_1 = q_1 = 0, \quad p'_1 = p_1 = 0, \quad (3\cdot17) \]
the \((q_2, p_2)\) plane itself is the collective submanifold. The orbit does not intersect with the plane \( q_1 = 0 \). In the case \( \theta = \pm 60^\circ \) we have
\[ q'_1 = \frac{1}{2}(q_1 \pm \sqrt{3}q_2) = 0, \quad p'_1 = \frac{1}{2}(p_1 \pm \sqrt{3}p_2) = 0. \quad (3\cdot18) \]

Putting \( q_1 = 0 \) in Eq. (3\cdot18) and in the energy equation
\[ E = \frac{1}{2}(q_1^2 + p_1^2 + q_2^2 + p_2^2) + q_1^2 q_2 - \frac{1}{3} q_2^3, \quad (3\cdot19) \]
we obtain invariant points \((q_2, p_2) = (0, \pm \sqrt{E/2})\) for \( \theta = \pm 60^\circ \).

For \( \theta = \pm 30^\circ \), putting \( q_1'' = 0, p_1'' = 0, q_1 = 0 \), we obtain

\[
\begin{align*}
 p_1 &= \mp \frac{3 + 2q_2}{\sqrt{3}(3 - 2q_2)} p_2, \\
 p_2^2 &= \frac{q_2^2 (2 - q_2)(3 - 2q_2)^2}{32}, \\
 E &= -\frac{1}{12} q_2^4 - \frac{1}{24} q_2^3 + \frac{1}{16} q_2^2 + \frac{3}{8} q_2.
\end{align*}
\]

(3\cdot20)

We may regard a solution as meaningful only when \( p_1, p_2 \) and \( q_2 \) are all real and their absolute values are sufficiently small compared with unity. For small energy the last equation has only one solution which fulfills the requirements. At \( E = 1/12 \), the invariant points are approximately found to be \((q_2, p_2) = (0.22, \mp 0.28)\) for \( \theta = \pm 30^\circ \).

For \( \theta = 90^\circ \), we obtain
Extraction of a Collective Submanifold

\[
\begin{align*}
\dot{q}_1 &= -\frac{3}{2} q_2 \left(1 + \frac{2}{3} q_2\right)^2, \\
\dot{q}_2 &= 0, \\
E &= -\frac{1}{12} q_3 (8 q_2^2 + 6 q_2 + 9),
\end{align*}
\] (3.21)

which approximately gives an invariant point \((q_2, p_2) \approx (-0.12, 0)\) at \(E = 1/12\).

[Type II]

The transformation (3.6) yields a new Hamiltonian

\[
H'(q', p') = \frac{1}{2} \left(\omega_1 (q_1^2 + p_1^2) + \omega_2 (q_2^2 + p_2^2)\right) + \delta_1 q_1^2 p_1 + \delta_2 p_1^3 + \delta_3 q_2 p_2^2 + \delta_4 q_2^3 \\
+ \epsilon_1 q_1' q_2' p_2' + \epsilon_2 p_1' p_2^2 + \epsilon_3 p_1' q_2^2 + \lambda_1 q_1' q_2' + \lambda_2 q_1' q_2' + \lambda_3 p_1' q_2'
\] (3.22)

with

\[
\begin{align*}
\delta_1 &= -\cos^2 \varphi \sin \varphi, & \epsilon_1 &= -2\cos^2 \varphi \sin \varphi, & \lambda_1 &= 2\cos \varphi \sin^2 \varphi, \\
\delta_2 &= -\frac{1}{3} \sin^3 \varphi, & \epsilon_2 &= -\sin^3 \varphi, & \lambda_2 &= \cos^3 \varphi, \\
\delta_3 &= \cos \varphi \sin^2 \varphi, & \epsilon_3 &= \cos^2 \varphi \sin \varphi, & \lambda_3 &= -\cos \varphi \sin^2 \varphi, \\
\delta_4 &= -\frac{1}{3} \cos^3 \varphi, & \omega_1 &= \omega_2 = 1.
\end{align*}
\] (3.23)

The transformation to a maximal decoupling form up to degree 3 is generated by

\[
W^{(3)}(q', p') = -\frac{1}{3} (a q_1' q_2'^2 + \beta q_1' p_2^2 + \gamma p_1' q_2'^2)
\] (3.24)

with

\[
\begin{align*}
a &= -\frac{3}{4} (c_1 + c_2 + c_3) = \varepsilon_1 + 2\varepsilon_2 + \varepsilon_3, \\
\beta &= -\frac{3}{4} (-c_1 + c_2 - c_3) = -\varepsilon_1 + \varepsilon_2 + 2\varepsilon_3, \\
\gamma &= -\frac{3}{2} (-c_1 + c_3) = \varepsilon_1 + 2\varepsilon_2 - 2\varepsilon_3, \\
c_1 &= -\varepsilon_1 + \varepsilon_2 - \varepsilon_3 \quad \omega_1 + 2\omega_2, & c_2 &= -\frac{2\varepsilon_2 - 2\varepsilon_3}{\omega_1}, & c_3 &= \frac{\varepsilon_1 + \varepsilon_2 - \varepsilon_3}{\omega_1 - 2\omega_2},
\end{align*}
\] (3.25)

and we have

\[
\begin{align*}
q_1'' &= q_1' - \frac{1}{3} \gamma q_2' p_2'', \\
p_1'' &= p_1' + \frac{1}{3} (a q_2'^2 + \beta p_2'^2),
\end{align*}
\]
\[ q_2'' = q_2' - \frac{1}{3}(2\beta q_1' p_2'' + \gamma p_1'' q_2'), \]
\[ p_2'' = p_2' + \frac{1}{3}(2\alpha q_1' q_2' + \gamma p_1'' p_2'). \]

In this case, the generating function \( W^{(4)} \) has divergent terms,
\[ W^{(4)}(\eta, \eta^*) = i\frac{g}{\omega_2 - \omega_1}(\eta \eta^* q_2' q_1') - i\frac{g^*}{\omega_2 - \omega_1}(\eta^2 \eta_1^*), \]
\[ q_k'' = \frac{1}{\sqrt{2}}(\eta_k + \eta_k^*), \quad p_k''' = -\frac{i}{\sqrt{2}}(\eta_k - \eta_k^*), \]
\[ \tilde{W}^{(4)}(\eta, \eta^*) = W^{(4)}(q'', p'''), \]
and we have
\[ g = -\frac{28}{3} i \cos \varphi \sin \varphi (1 - 2\cos^2 \varphi). \]

It vanishes at \( \varphi = 0^\circ, \pm 45^\circ, 90^\circ \). \( (-90^\circ < \varphi \leq 90^\circ) \)

The case \( \varphi = 0^\circ \) is identical with \( \theta = 0^\circ \).

For \( \varphi = \pm 45^\circ \), we obtain
\[
\begin{cases}
    p_1 = \pm \sqrt{(2 - q_2) - \sqrt{4 - 8q_2}}, \\
    p_2 = 0, \\
    E = \frac{1}{2} \left[ ((2 - q_2) - \sqrt{4 - 8q_2})^2 + q_2^2 - \frac{2}{3} q_2^3 \right].
\end{cases}
\]

The invariant points are approximately found to be \((q_2, p_2) \approx (0.25, 0)\) for \( \varphi = 45^\circ \) and \((-0.31, 0)\) for \( \varphi = -45^\circ \) at \( E = 1/12 \), corresponding to C and D in Fig. 1. Although three other sets of equations also appear, they have no acceptable solutions.

For \( \varphi = 90^\circ \), we obtain
\[
\begin{cases}
    p_1^2 = -\frac{3}{2}q_2, \\
    p_2 = 0, \\
    E = \frac{1}{12} \left( -9q_2 + 6q_2^2 - 4q_2^3 \right),
\end{cases}
\]

which approximately gives an invariant point \((q_2, p_2) \approx (-0.10, 0)\) at \( E = 1/12 \), identified with that for \( \theta = 90^\circ \) which gives \((q_2, p_2) \approx (-0.12, 0)\). The small discrepancy in the numerical values has been caused by an ambiguity in the transformation to a maximal-decoupling form up to degree 3, and is considered to become smaller and smaller as the transformation is repeated. Another set of equations also appears without any acceptable solution.

Through the above argument, the collective submanifolds are maximally decoupled with respect to the variables with suffix 1. The maximal-decoupling procedure
with respect to the variables with suffix 2 leads to the same results only with the difference of the angles, for which \( h \) and \( g \) vanish, by 90°.

The obtained invariant points are summarized in Table I.

§ 4. Summary and discussion

In this paper, we have applied the procedure for maximally decoupling a collective submanifold to the Hénon-Heiles system and we have obtained periodic orbits. An infinite number of modes exist with neglect of the third-order terms. We have decided which modes survive with the third-order terms from the condition that the terms with zero denominators vanish in the generating functions \( W(6) \) for Type I and \( W(4) \) for Type II, which induce maximally-decoupled Hamiltonian. Those modes are expected to be maximally decoupled up to infinite degree. The locations of the invariant points in the Poincaré mapping corresponding to them have been calculated and are in good agreement with the numerical results by computer simulation.*

This method, however, has a problem. The generating function cannot be uniquely determined. For example, we can add to \( W(3)(q', p') \) the following terms:

\[
\rho_1 q_2 q_2 q_1 + \rho_2 q_2 q_2 q_1^2 + \rho_3 q_1 q_2 + \rho_4 q_1 q_2^2 q_1 + \rho_5 q_2 q_1^2 \\
+ \rho_6 q_1 q_2 + \rho_7 q_1 q_2 q_2^3 + \rho_8 q_1^3 q_2 + \rho_9 q_1^3 q_2^3,
\]

where \( \rho_k \) can take any value. The conditions for \( \theta \) and \( \varphi \) are shown to be independent of the parameters \( \rho_k \). The locations of invariant points, however, are not. It might be hoped that this ambiguity would disappear if we repeat the decoupling procedure to higher orders, but this is not the case. This non-uniqueness is somewhat embarrassing in view of the consistency of the present results with the computer simulation. In this paper we have chosen a generating function which has only the minimal terms. It would be a reasonable choice.

Another possible way to get rid of this problem is to use

\[
\begin{align*}
q_k'' &= q_k' + \frac{\partial W^{(3)}(q', p')}{\partial p_k''}, \\
p_k'' &= p_k' - \frac{\partial W^{(3)}(q', p')}{\partial q_k''}, \\
W^{(3)} &= W^{(3)} + (4\cdot1),
\end{align*}
\]

(4·2)

consistently with decoupling up to degree 3, rather than the "exact" equations

\[
\begin{align*}
q_k'' &= q_k' + \frac{\partial W^{(3)}(q', p')}{\partial p_k''}, \\
p_k'' &= p_k' - \frac{\partial W^{(3)}(q', p')}{\partial q_k''}
\end{align*}
\]

(4·3)

for determining the locations of invariants points. Putting \( q_i'' = p_i'' = 0 \) automatically

\( * \) All the simple periodic orbits have been obtained by the present method, while non-simple periodic orbits represented by a finite number of invariant points have not.
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leads to a unique solution.\textsuperscript{(*)} The locations of invariant points obtained in this way are slightly different but still lie near the values in Table I. In any case, this problem has not been satisfactorily solved.

Finally we suggest an interesting situation which has something to do with the present analysis on the relation between survival of the modes and divergence of the power series. Let us consider a system of two nonlinearly interacting oscillators with $\omega_2 - n_0 = \Delta$ or $\omega_1 - n_\omega = \Delta (n=1, 2, \cdots; |\Delta| < 1)$. We have at least two periodic orbits with neglect of terms of order higher than the quadratic. With the higher-order terms involved, the power series are expected to converge and the periodic orbits still exist for small energy. Above some energy point, however, the power series will generally diverge since the generating functions involve the factor $1/|\Delta|$ and the corresponding collective submanifold will disappear. The periodic orbit will get transformed into a quasi-periodic one or an ergodic one. For example, let us take the Hénon-Heiles-like system (3·7) with $2\omega_2 - \omega_1 = \Delta$ ($0 < |\Delta| < 1$). From Eq. (3·11) the variables $q_s^{**}$ and $p_s^{**}$ are written down in the form of power series in $q_s'$ and $p_s'$, which diverge above some critical energy. With neglect of the third-order terms, we have two periodic orbits corresponding to $\theta = 0^\circ$ and $\theta = 90^\circ$. The latter will cease to be periodic from the above argument, while the former will remain it below the escape energy\textsuperscript{3} since it is maximally decoupled without a transformation from $(q_s', p_s')$ to $(q_s'', p_s'')$. This conjecture can be straightforwardly extended to the system consisting of many oscillators. It is an interesting question how such a behavior of the collective submanifold appears in nuclei.\textsuperscript{81}

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Appendix

The generating functions $W^{(4)}$ and $W^{(5)}$ for Type I are given here. Using the relations $3\mu_3 = -\nu_2$ and $3\mu_2 = -\nu_1$, we have

\begin{equation}
W^{(4)}(q^*, p^*) = 3\mu_1\mu_2(-p_2^{**}q_1 + p_2^{**}q_2 p_1^{**} + p_2^{**}q_3 p_1^{**} - q_2^{**}p_1^{**})
\tag{A·1}
\end{equation}

and

\begin{equation}
W^{(5)}(q^{(3)}, p^{(4)}) = \mu_1(-54\mu_2^2p_2^4p_1 - 4\mu_2^4p_1 - 54\mu_2^2p_2^3q_3q_1 - 104\mu_2^2p_2^3q_3q_1 - 81\mu_2^2p_2^3q_3q_1 + 64\mu_2^2p_2^2q_3q_1 + 156\mu_2^2p_2^2q_3q_1 - 96\mu_2^2p_2^2q_3q_1 + 21\mu_2^2p_2^2q_3q_1 + 71\mu_2^2p_2^2q_3q_1),
\tag{A·2}
\end{equation}

\textsuperscript{(*)} This procedure is not enough for $p_\rho$ and $p_{\rho_0}$ terms, but these terms essentially generate a canonical transformation among the $(q_s^*, p_s^*)$ which are decoupled from $(q_s', p_s')$. 


where \( q_k \) and \( p_k \) on the right-hand side of (A·2) denote \( q_k^{(3)} \) and \( p_k^{(4)} \), respectively.

References

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