HIGHER ORDER SYMPLECTIC METHODS BASED ON MODIFIED VECTOR FIELDS

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ABSTRACT

HIGHER ORDER SYMPLECTIC METHODS BASED ON MODIFIED VECTOR FIELDS

The higher order, structure preserving numerical integrators based on the modified vector fields are used to construct discretizations of separable systems. This new approach is called as modifying integrators. Modified vector fields can be used to construct high-order, structure-preserving numerical integrators for ordinary differential equations. In this thesis by using this approach the higher order symplectic numerical methods based on symplectic Euler method are obtained. Stability and consistency analysis are also studied for these new higher order numerical methods. Finally the proposed new numerical schemes applied to the separable Hamilton systems.

ÖZET

UYARLANABİLEN VEKTÖR ALANLARI KULLANILARAK YÜKSEK MERTEBEDEN SİMPLEKTİK METODLARIN ELDE EDİLMESİ

Uyarlanabilen vektör alanları kullanılarak elde edilen yüksek mertebeden, yapı koruyan nümerik yöntemler ayrık sistemlerin diskritizasyonunda kullanılmaktadır. Bu yeni yaklaşım uyarlanabilir entegratörler olarak adlandırılmaktadır. Uyarlanabilen vektör alanları adi diferansiyel denklemler için yüksek mertebeden, yapı koruyan nümerik entegratörler elde etmek için kullanılabilmektedir. Bu yaklaşıma dayanarak, bu tezde simplektik Euler yöntemi temel alınarak yüksek mertebeden, simplektik metodlar elde edilmiştir. Bununla birlikte elde edilen bu yeni yöntemlerin kararlılık ve tutarlılık analizleri üzerinde de çalışılmıştır. Son olarak elde edilen bu yeni metodlar ayrılabilir Hamilton sistemlere uygulanmıştır.

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CHAPTER 1

INTRODUCTION

During the past decade there has been an increasing interest in studying numerical methods that preserve certain properties of some differential equations (Budd and Piggott 2000). In recent years, geometric numerical integration methods have come to the fore, partly as an alternative to traditional methods such as Runge-Kutta methods. A numerical method is called *geometric integrator* if it preserves one or more physical/geometric properties of the system exactly (i.e up to round-off error). Examples of such geometric properties that can be preserved are (first) integrals, symplectic structure, symmetries and reversing-symmetries, phase-space volume, Lyapunov functions, foliations, e.t.c. Geometric methods have applications in many areas of physics, including celestial mechanics, particle accelerators, molecular dynamics, fluid dynamics, pattern formation, plasma physics, reaction-diffusion equations, and meteorology.

Probably the first significant area where geometric ideas were used was in the (symplectic) integration of Hamiltonian ordinary differential equations. Hamilton systems form the most important class of ordinary differential equations in the context of geometric integration. An outstanding property of Hamilton systems is the symplecticity of the flow. The name symplectic integrator is usually attached to a numerical scheme that intends to solve such a hamiltonian system approximately, while preserving its underlying symplectic structure. Symplectic integrators tend to preserve qualitative properties of phase space trajectories: trajectories do not cross, and although energy is not exactly conserved, energy fluctuations are bounded. First examples of symplectic integrators are implicit midpoint rule, Strmer-Verlet methods, some Runge Kutta methods such as Gauss Collocation and Lobatto IIIA-IIIB methods.

In the literature symplectic methods are generally constructed using generating functions, Runge Kutta methods, splitting methods and variational methods. One of the methods for constructing high-order symplectic integrators is developed by using modified vector fields. The primary work on this approach was developed by Philippe Chartier, Ernst Hairer and Gilles Vilmart(Chartier, et al. 2006) and illustrated by the implicit midpoint rule applied to the full dynamics of the rigid body. Roman Kozlov used the idea of

modified vector field in his paper, ”Higher-order conservative discretization of the three dimensional Kepler motion”(Kozlov 2007) as well. This approach is developed by using the idea in backward error analysis while constructing modified equations by inverting the roles of the exact and numerical flows.

In this thesis we construct new higher order symplectic methods based on symplectic Euler method inspired by the theory of modified vector fields in combination with backward error analysis.

The outline of this thesis can be given as follows: After giving the idea of modified equations in combination with backward error analysis in Chapter 2. We give the idea of modifying integrators, introduce symplectic integrators and construct new higher order symplectic numerical method in Chapter 3. Order of accuracy, consistency, stability analysis of the proposed numerical methods are studied in Chapter 4. Finally in Chapter 5, these new methods are applied to separable Hamilton systems namely Harmonic Oscillation and Double Well systems.

CHAPTER 2

BACKWARD ERROR ANALYSIS AND MODIFIED EQUATIONS

In this chapter we introduce some important keywords that will be useful for the next chapters. Since the topic of this thesis is the numerical integrators based on the modified vector fields we have to give the definition of modified differential equations in combination with backward error analysis.

2.1. Backward Error Analysis

The general concept of backward error analysis was developed and used extensively by Wilkinson in his work during the 1950s and 1960s, primarily in the field of numerical linear algebra (Wilkinson 1963). For the study of integration methods for ordinary differential equations it's importance was seen much later. Backward error analysis is very useful, when the qualitative behavior of numerical methods is of interest, and when statements over very long time intervals are needed. The formal analysis (construction of the modified equation, study of its properties) gives already a lot of insight into the numerical methods. For a rigorous treatment, the modified differential equation, which is a formal series in powers of the step-size, has to be truncated. The error, induced by such truncation, can be made exponentially small, and the results remain valid on exponentially long time intervals. (Hairer, et al. 2002)

Now the idea of modified differential equations in the content of backward error analysis can be given.

2.2. Modified Equations for Backward Error Analysis

Modified differential equations in combination with backward error analysis form an important tool for studying long-time behavior of numerical integrators for ordinary differential equations. A modified equation is a truncated series in powers of step size, that is solved to higher order by a numerical scheme. Such a transformation induces an error

which can be made exponentially small, and the results remain valid on exponentially long time intervals. It is very useful when the qualitative behavior of a numerical scheme is of interest, and when statements over long time intervals are needed.

The idea of modified equations is to describe a numerical solution as points along the exact solution of a modified problem which is in some sense near the original problem. That is, the *exact* solutions of the modified problem "interpolate" the numerically approximated solution. The word interpolate is used loosely, and should be thought of as meaning merely that for a given fixed time step h, the modified solution passes through the points of the numerical solution. For large h, the modified solutions may vary wildly between points of the numerical solution and do not necessarily provide a good or natural interpolant to the numerical solution in the traditional sense.

Though notions of backward analysis and backward stability of problems has been around for some time, the method of modified equations as a means of (backward) analyzing numerical solutions of differential equations is a much more recent development.

The primary motivation for seeking such modified problems is that frequently they are easier to understand than the discrete dynamical systems (i.e. difference equations) which define the numerical integrator. In essence, they are useful because models are usually developed and expressed in terms of continuous systems which are difficult to compare with discrete maps. However, modified equations can also prove useful in obtaining long-term estimates of quantities defined strictly by discrete models with maps sufficiently close to the identity.

Backward error analysis has a history of succeeding where forward analysis fails. Wilkinson's classical result regarding the stability of Gaussian elimination could not be explained through the traditional forward analysis approach (Wilkinson 1961). Modified equations have been used to explain the success of numerical methods applied to chaotic systems and perhaps most notably they have been used to prove a series of theorems regarding the structure preservation of certain types of methods (e.g. energy conservation of symplectic methods). Briefly, these theorems are of the form, "if the system is Hamiltonian and the method is symplectic, then the modified system is also Hamiltonian". A similar statement holds with Hamiltonian and symplectic replaced by reversible and symmetric respectively. The proof of these statements is by induction and can be found in (Hairer and Stoffer 1997), (Hairer 1984) and (Hairer, et al. 2002).

2.2.1. Construction of the Modified Equation

Consider an ordinary differential equation

$$\dot{y} = f(y), \;\; y(0) = y_0 \tag{2.1}$$

with sufficiently smooth vector field $f(y)$, and the numerical method $\Phi_{f,h}(y)$ applied to (2.1) which produces the approximations $y_0, y_1, y_2, ...$ such that

$$y_{n+1} = \Phi_{f,h}(y_n) \tag{2.2}$$

A forward error analysis consists of the study of errors $y_1 - \varphi_h(y_0)$ (local error) and $y_n - \varphi_{nh}(y_0)$ (global error) in the solution space where φ is the exact flow of (2.1). The idea of backward error analysis is to search a modified equation $\dot{\tilde{y}} = f_h(\tilde{y})$ of the form

$$\dot{\tilde{y}} = f_h(\tilde{y}) = f(\tilde{y}) + hf_2(\tilde{y}) + h^2 f_3(\tilde{y}) + ..., \quad \tilde{y}(0) = y_0, \tag{2.3}$$

such that $y_n = \tilde{y}(nh)$, and in studying the difference of the vector fields $f(y)$ and $f_h(y)$. This then gives much insight into the qualitative behavior of numerical solution and into the global error $y_n - y(nh) = \tilde{y}(nh) - y(nh)$.

We seek a perturbed or modified function f_h such that the solution $\tilde{y}$, of $\dot{\tilde{y}} = f_h(\tilde{y})$ matches the solution of (2.2) at the points $t = 0; h; 2h; .....$

We remark that the series in (2.3) usually diverges and that one has to truncate it suitably. The effect of such a truncation will be given with a theorem after giving the idea of modified differential equations.

The below figure illustrates this idea.

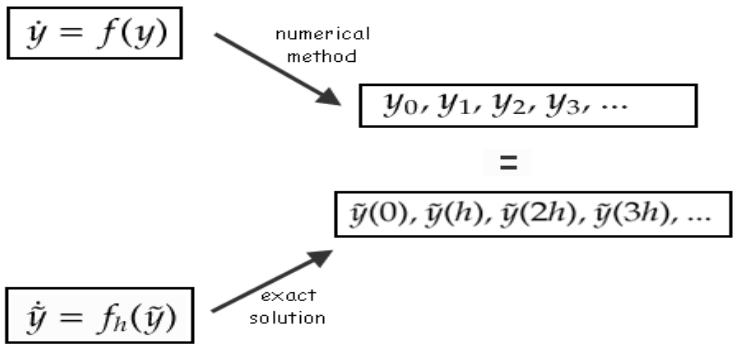

Figure 2.1. Idea of Backward Error Analysis with Modified Differential Equations.

In general, it is not possible to obtain an expression for f_h explicitly. Instead f_h can be written as a formal series in powers of h, with the terms defined recursively. This series does not converge in general but suitable truncations of the series can approximate f_h well. There are several approaches for calculating the terms in the h-expansion of f_h. Here we closely follow the approach of Hairer (Hairer, et al. 2002). The idea is to take expansions of $\tilde{y}$ and $\Phi_{f,h}$ and match terms of equal powers of h. For the computation of the modified equation (2.3) we put $y := \tilde{y}(t)$ for a fixed t, and expand the solution of (2.3) into a Taylor series

$$\begin{aligned}
\tilde{y}(t+h) &= \tilde{y}(t) + h\dot{\tilde{y}}(t) + \frac{h^2}{2}\ddot{\tilde{y}}(t) + \frac{h^3}{3!}\tilde{y}^{(3)}(t) + ... \\
&= \tilde{y}(t) + hf_h + \frac{h^2}{2}f_h' f_h + \frac{h^3}{3!}(f_h''(f_h, f_h) + f_h' f_h' f_h) \\
&= y + h(f + hf_2 + h^2 f_3 + ...) \\
&+ \frac{h^2}{2!}(f' + hf_2' + h^2 f_3' + ...)(f + hf_2 + h^2 f_3 ...) + ... \\
&= y + hf + h^2(f_2 + \frac{1}{2!}f'f) + h^3((f_3 + \frac{1}{2!}(f_2' f + f' f_2) \\
&+ \frac{1}{3!}(f''(f,f) + f'f'f)) + ... \qquad (2.4)
\end{aligned}$$

Here f, f', f'' represent $f(y), f'(y), f''(y)$ respectively. Also note that f' is the Jacobian of f and f'' ,$f^{(3)}$... binary,ternary operators taking 2,3,... arguments. Term by term comparison of (2.4) to the expansion of $\Phi_{f,h}$

$$\Phi_{f,h}(y) = y + hf(y) + h^2 d_2(y) + h^3 d_3(y) + ..., \qquad (2.5)$$

gives the functions f_{k+1} in terms of the $f_2, f_3, ...f_k$

$$\begin{aligned}
f_2 &= d_2 - \frac{1}{2!}f'f, \\
f_3 &= d_3 - \frac{1}{3!}(f''(f,f) + f'f'f) - \frac{1}{2!}(f'f_2 + f_2' f), etc. \qquad (2.6)
\end{aligned}$$

Methods for implementing this recursion are given by Hairer (Hairer, et al. 2002) and by Ahmed and Corless (Ahmed and Corless 1997) among others. For most functions f,the symbolic computations become very costly for higher order terms. An elegant represen-

tation of the recurrence relation can by achieved through the use of trees and ordered trees (Hairer, et al. 2002), but will not be presented here as it is outside the scope of this work.

A very similar approach is taken by Reich (Hairer 1999) to develop an expression for the modified equation, the main difference there being that a recursive expression is written to define the terms $f_2, f_3, \ldots$ of the modified equation (i.e. f_{i+1} is defined in terms of f_i). The approach is exactly the same otherwise but may be advantageous in the practical construction of modified equations. With the development of symbolic computing packages such as Maple, the often cumbersome task of computing terms of the modified equation can be fully automated. There are several published codes for symbolically computing modified equations in Maple (Ahmed and Corless 1997) and (Hairer, et al. 2002).

Example 2.1 *Consider the scalar differential equation*

$$\dot{y} = y^2, \qquad y(0) = 1$$

with exact solution $y(t) = \frac{1}{1-t}$. *It has a singularity at t=1. The exact solution exists for* $t < 1$. *We apply the explicit Euler method* $y_{n+1} = y_n + hf(y_n)$. *The one term modified differential equation (MDE-1) is*

$$\dot{\tilde{y}} = f(\tilde{y}) - \frac{h}{2} f'(\tilde{y}) f(\tilde{y}) = \tilde{y}^2 - h\tilde{y}^3 \tag{2.7}$$

The system has an unstable equilibrium at $y = 0$ *and an asymptotically stable equilibrium at* $y = \frac{1}{h}$. *In particular a solution exists for all time. The Figure (2.2) shows the exact solution,the forward euler solution and the modified equation solution for* $h = 0.1$ *The modified equation is not much closer to the numerical solution than the exact solution is, but it does exist for all time.*

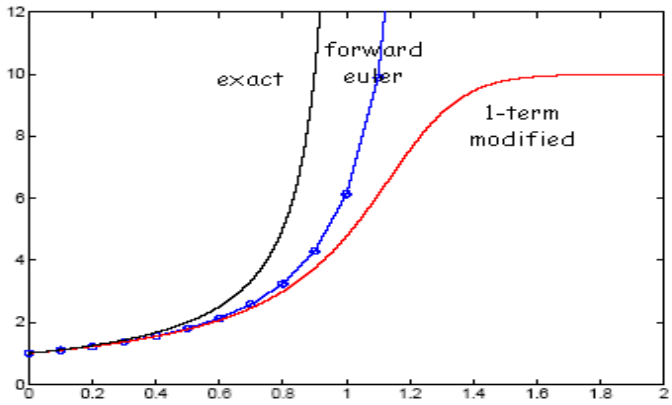

Figure 2.2. Exact, Forward Euler and MDE-1 Solutions to $\dot{y} = y^2, y(0) = 1$.

Continuing the procedure outlined above to determine higher order terms(and making use of symbolic mathematics software) gives the five term modified equation. Its output is

$$\dot{\tilde{y}} = \tilde{y}^2 - h\tilde{y}^3 + \frac{3}{2}h^2\tilde{y}^4 - \frac{8}{3}h^3\tilde{y}^5 + \frac{31}{6}h^4\tilde{y}^6 - \frac{157}{15}h^5y^7 \mp .... \tag{2.8}$$

The Figure(2.3) presents the exact solution, the Forward Euler method and m-term modified equations (MDE-m) for $m = 1, ..., 5$ plotted for $h = .02$. We see that the modified equation solutions 'converge' to the numerical solution very quickly as h become smaller. We observe an excellent agreement of the numerical solution with the exact solution of the modified equation.

By the similar way the modified equation w.r.t midpoint rule can be obtained given as below

$$\dot{\tilde{y}} = \tilde{y}^2 + \frac{1}{4}h^2\tilde{y}^4 + \frac{1}{8}h^4\tilde{y}^6 + \frac{11}{192}h^6\tilde{y}^8 + \frac{3}{128}h^8\tilde{y}^{10} \mp .... \tag{2.9}$$

For the classical Runge-Kutta method of order 4

$$\dot{\tilde{y}} = \tilde{y}^2 - \frac{1}{24}h^4\tilde{y}^6 + \frac{65}{576}h^6\tilde{y}^8 - \frac{17}{96}h^7\tilde{y}^9 + \frac{19}{144}h^8\tilde{y}^{10} \mp .... \tag{2.10}$$

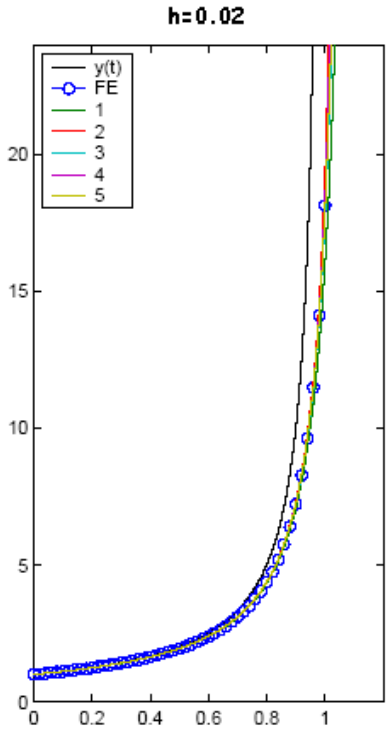

Figure 2.3. Exact,Forward Euler and MDE-m Solutions to $\dot{y} = y^2, y(0) = 1$.

We observe that the perturbation terms in modified equation are of size $O(h^p)$, where p is the order of the method. This is true in general.

Theorem 2.1 *Suppose that the method $y_{n+1} = \phi_{f,h}(y_n)$ is of order p, i.e.,*

$$\phi_{f,h}(y_n) = \varphi_h(y) + h^{p+1}\delta_{p+1}(y) + O(h^{p+2})$$

where $\varphi_t(y)$ denotes the exact flow of $\dot{y} = f(y)$, and $h^{p+1}\delta_{p+1}(y)$ the leading term of the local truncation error. The modified equation then satisfies

$$\dot{\tilde{y}} = f(\tilde{y}) + h^p f_{p+1}(\tilde{y}) + h^{p+1} f_{p+2}(\tilde{y}) + \ldots, \quad \tilde{y}(0) = y_0 \tag{2.11}$$

with $f_{p+1}(y) = \delta_{p+1}(y)$.

Proof: The construction of the functions $f_j(y)$ (see the beginning of this section) shows that $f_j(y) = 0$ for $2 \le j \le p$ if and only if $\phi_{f,h}(y) - \varphi_h(y) = O(h^{p+1})$.

A first application of the modified equation (2.3) is the existence of an asymptotic expansion of the global error. Indeed by the nonlinear variation of constants formula, the difference between its solution $\tilde{y}(t)$ and the solution $y(t)$ of $\dot{y} = f(y)$ satisfies

$$\tilde{y}(t) - y(t) = h^p e_p(t) + h^{p+1}(t) + \ldots \tag{2.12}$$

Since $y_n = \tilde{y}(nh) + O(h^N)$ for the solution of a truncated modified equation, this proves the existence of an asymptotic expansion in powers of h for the global error $y_n - y(nh)$.

In general, the series (2.3) diverges and the infinite order modified equation does not exist. Nonetheless, taking a finite number of terms of the series (2.3) yields a truncated modified equation that can still provide a good approximation to the behavior of the discrete dynamical system.

Consider the truncated modified differential equation

$$\dot{\tilde{y}} = F_N(\tilde{y}), \qquad F_N(\tilde{y}) = f(\tilde{y}) + hf_2(\tilde{y}) + ... + h^{N-1}(\tilde{y}) \tag{2.13}$$

There exists an optimal value of m, dependent on h and denoted by N for which the difference between the m-term modified equation and the numerical solution is minimized. N increases like $1/h$ as h tends to zero, and usually much larger than the order p of the numerical method. In other words, the modified equations are indeed a useful tool in understanding numerical methods.

Theorem 2.2 *Let $f(y)$ be analytic in a complex neighborhood of y_0 and that $||f(y)|| \leq M$ for $||y - y_0|| \leq 2R$ i.e., for all y of $\mathcal{B}_{2R}(y_0) := \{y \in \mathbb{C}^d; ||y - y_0|| \leq 2R\}$, let the coefficients $d_j(y)$ of the method (2.5) be analytic and bounded in $\mathcal{B}_R(y_0)$. If $h < h_0/4$ where $h_0 \propto R/M$ then there exists $N = N(h)$ (namely N equal to the largest integer satisfying $hN \leq h_0$)such that the difference between the numerical solution $y_1 = \phi_h(y_0)$ and the exact solution $\tilde{\varphi}_{N,t}(y_0)$ of the truncated modified equation (2.13) satisfies*

$$||\phi_h(y_0) - \tilde{\varphi}_{N,h}(y_0)|| \leq h\gamma M e^{-h_0/h}, \tag{2.14}$$

Proof: See (Hairer, et al. 2002).

2.3. Geometric Properties

The importance of backward error analysis in the context of geometric numerical integration lies in the fact that properties of numerical integrators are transferred to corresponding properties of modified equations.Because of the close relationship between backward error analysis and the approach of modifying integrators, it is not a surprise that most results can be extended to our situation. The most important properties of the modified equation can be collected given as below:

• If the numerical integrator $\Phi_{f,h}(y)$ has order p, i.e., the local error satisfies $\Phi_{f,h}(y) - \varphi_{f,h}(y) = O(h^{p+1})$, then we have $f_j = 0$ for $j = 2, ..., p$;

• If the numerical integrator $\Phi_{f,h}(y)$ is symmetric, i.e, $\Phi_{f,-h}(y) = \Phi^{-1}_{f,h}(y)$, then the modified differential equation has an expansion in even powers of h, i.e., $f_{2j} = 0$ for all j, and modifying integrator is symmetric.

• If the basic method $\Phi_{f,h}(y)$ exactly conserves a first integral $I(y)$ of (2.1), then the modified differential equation has $I(y)$ as first integral, and the modifying integrator exactly conserves $I(y)$.

• If the basic method is symplectic for Hamiltonian systems of the form $\dot{y} = J^{-1}\nabla\tilde{H}(y)$; the modifying integrator is also

• If the basic method is reversible for reversible differential equations then the modified differential equation and the modifying integrator are reversible;

The proofs of these properties can be found in (Hairer, et al. 2002). Here we are not concerned with these proofs.

CHAPTER 3

HIGHER ORDER SYMPLECTIC METHODS BASED ON MODIFIED VECTOR FIELDS

3.1. Modifying Numerical Integrators

Motivated by the theory of modified differential equations(backward error analysis) an approach for construction of higher order numerical integrators that preserve geometric properties of the exact flow is developed. This integrators are called modified integrators.

The main idea of the theory of modified integrators is sketched by inverting the roles of the ”numerical method” and the ”exact solution”, it can be turned into a means by constructing high order integrators that conserve geometric properties. They will be useful for integrations over long times. This method was used by Philippe Chartier, Ernst Hairer and Gilles Vilmart in the equations of motion for a rigid body as a numerical integrator they have chosen the Discrete Moser-Veselov algorithm (DMV)(Moser and Veselov 1991).Also Roman Kozlov used this method in his work called conservative discretizations of the Kepler motion (Kozlov 2007).

As before, we consider an ordinary differential equation (2.1) and a numerical integrator(2.2). But now we search for a modified differential equation again of the form (2.3), such that the numerical solution $\tilde{y}_n$ of the method applied with step size h to (2.3) yields formally the exact solution of the original equation (2.1),i.e.,

$$\tilde{y}_n = y(nh) \quad for\, n = 0, 1, 2, ..., \tag{3.1}$$

The following figure illustrates this idea.

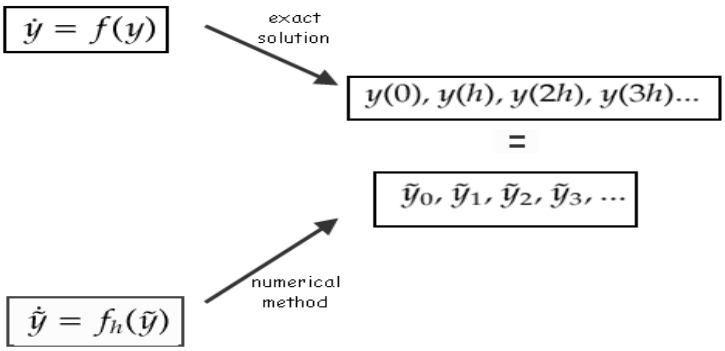

Figure 3.1. Idea of Modifying Numerical Integrators.

Notice that this modified equation is different from the one considered before. However because of the close connection with backward error analysis, all theoretical and practical results have their analogue in this new context. The modified differential equation is again an asymptotic series that usually diverges, and its truncation inherits geometric properties of the exact flow if a suitable integrator is applied. The coefficient functions f_j can be computed recursively by using a formulae manipulation program like MAPLE. Here the idea of obtaining a few of these coefficient functions will be given.

3.2. Construction of the Modifying Integrator

Consider the ordinary differential equation (2.1) and a numerical method (2.2). We again search for a modified differential equation (2.3) such that the numerical solution $\tilde{y}_n$ of the method applied with step size h to (2.3) yields formally the exact solution of the original differential equation (2.1), i.e. $\tilde{y}_n = y(nh)\ for\ \ n = 0,1,2,\ldots$. The coefficient functions f_j can be computed recursively.

Having found first functions f_j, one can use truncation for $r > 1$

$$\dot{\tilde{y}} = f_h^{[r]}(\tilde{y}) = f(\tilde{y}) + hf_2(\tilde{y}) + \ldots + h^{r-1}f_r(\tilde{y}) \tag{3.2}$$

of the modified differential equation corresponding to $\Phi_{f,h}(y)$. A numerical method $\tilde{y}_{n+1} = \Phi_{f_h^{[r]},h}(\tilde{y_n})$ approximates the solution of (2.1) with order r. It was called a *modifying integrator* because it applies to the modified vector field $f_h^{[r]}$ instead of $f(y)$.

This is an alternative approach for constructing high order numerical integrators for ordinary differential equations (classical approaches are multistep, Runge-Kutta,Taylor series,composition and splitting methods). It is particularly interesting in the context of geometric integration because, as known from backward error analysis, the modified differential equation inherits the same structural properties as (2.1) if a suitable integrator is applied.

Modifying integrators will be efficient when the evaluation of the truncated vector field in (3.2) is not much more expensive than that of $f(y)$. McLachlan (McLachlan 2007)discusses situations (N-body problems, lattice systems) where the computation of derivatives is cheap when it is performed together with the evaluation of $f(y)$. In this situations the modifying integrators have a large potential.

3.3. Construction of the Modifying Midpoint Rule

For the numerical integration of (2.1) we consider the implicit midpoint rule

$$y_{n+1} = y_n + h\, f(\frac{y_n + y_{n+1}}{2}) \tag{3.3}$$

We find the functions $f_j(y)$ of the truncated modified vector field with respect to implicit midpoint rule.

Consider the truncated modified differential equation (3.2)

$$\dot{\tilde{y}} = \underbrace{f_h^{[r]}(\tilde{y}) = f(\tilde{y}) + hf_2(\tilde{y}) + ... + h^{r-1}f_r(\tilde{y})}_{F} \tag{3.4}$$

and the Taylor expansion of exact solution $y(t)$ over h

$$y(t+h) = y(t) + hy\dot{(}t) + \frac{h^2}{2!}y\ddot{(}t) + \frac{h^3}{3!}y^3(t) + ..., \tag{3.5}$$

where $\ddot{y} = f'f$, $y^{(3)} = f'f'f + f''(f,f)$ and $\tilde{y}_{n+1} = \phi_{f_h^{[r]},h}(\tilde{y}_n)$ where the method here is midpoint rule

$$\begin{aligned}
\tilde{y}_{n+1} &= \tilde{y}_n + hF(\frac{\tilde{y}_n + \tilde{y}_{n+1}}{2}) \\
&= \tilde{y}_n + hF(\frac{\tilde{y}_n + \tilde{y}_n + hF(\frac{\tilde{y}_n + \tilde{y}_{n+1})}{2}}{2}) \\
&= \tilde{y}_n + hF(\tilde{y}_n + \frac{h}{2}F(\frac{\tilde{y}_n + \tilde{y}_{n+1}}{2})) \\
&= \tilde{y}_n + h[F(\tilde{y}_n) + \frac{h}{2}F(\frac{\tilde{y}_n + \tilde{y}_{n+1}}{2})\, F'(\tilde{y}_n) + \frac{h^2}{8}F^2(\frac{\tilde{y}_n + \tilde{y}_{n+1}}{2})\, F''(\tilde{y}_n) + ...] \\
&= \tilde{y}_n + hf + h^2[f_2 + \frac{1}{2}ff'] + h^3[f_3 + \frac{1}{2}f_2f' + \frac{1}{4}f'f'f + \frac{1}{8}f''(f,f)] + ...
\end{aligned} \tag{3.6}$$

Now equating the terms of (3.6) to the terms of the exact solution (3.5) expanded by Taylor series we get

$$f_2 + \frac{1}{2}f'f = \frac{1}{2}f'f \qquad \Rightarrow f_2 = 0 \tag{3.7}$$

$$f_3 = \frac{1}{12}(-f'f'f + \frac{1}{2}f''(f,f)) \tag{3.8}$$

$$f_4 = 0 \tag{3.9}$$

$$\begin{aligned} f_5 &= \frac{h^4}{120}(f'f'f'f'f - f''(f,f'f'f) + \frac{1}{2}f''(f'f,f'f)) \\ &+ \frac{h^4}{120}(-\frac{1}{2}f'f'f''(f,f) + f'f''(f,f'f) + \frac{1}{2}f''(f,f''(f,f)) - \frac{1}{2}f^{(3)}(f,f,f'f)) \\ &+ \frac{h^4}{80}(-\frac{1}{6}f'f^{(3)}(f,f,f) + \frac{1}{24}f^{(4)}(f,f,f,f)). \end{aligned} \tag{3.10}$$

We will give numerical application examples about modifying midpoint integrator as a numerical experiment for Harmonic Oscillator in chapter 5.

3.4. Construction of the Higher Order Symplectic Methods

At the beginning of this section we give some preliminary information about Hamiltonian systems and symplectic methods .

3.4.1. Hamiltonian Systems

Probably the first significant area where geometric ideas were used was in the (symplectic) integration of Hamiltonian ordinary differential equations. This is natural as Hamiltonian systems often have very important applications in mechanics, celestial and molecular dynamics and optics and their analysis, since Hamilton's original papers has always centered on the geometric structure of the equation. The numerical methods for solving such systems are called symplectic methods that will be given in the following subsections.

The Theory of Hamiltonian Methods:

Consider initially a mechanical system with generalized coordinates $q \in \mathcal{R}^d$ and Lagrangian $L = T - V$ where $T \equiv T(q,\dot{q})$ represents the kinetic energy of the system and $V \equiv V(q)$ represents the potential energy. The dynamics of such a system can be studied in terms of the calculus of variations by considering the action function is constructed

by integrating L along a curve $q(t)$ and then computing variations of the action while holding the end points of the curve $q(t)$ fixed. The details are given in (Marsden and West 2001). It can be shown easily that this procedure leads to following Euler-Lagrange equations describing the motion

$$\frac{d}{dt}(\frac{\partial L}{\partial \dot{q}}) - \frac{\partial L}{\partial q} = 0 \tag{3.11}$$

Hamilton recognized that these equations could be put into a form which allowed a more geometrical analysis. In particular he introduced the coordinates

$$p = \frac{\partial L}{\partial \dot{q}} \in \mathcal{R}^d \,, \tag{3.12}$$

which are conjugate generalized momenta for the system. He further defined the Hamiltonian via a Legendre transformation as

$$H(q,p) = p^T \dot{q} - L(q,\dot{q}) \tag{3.13}$$

and showed that (3.11) is equivalent to the following system of *2d* first-order equations, called Hamilton's equations.

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \tag{3.14}$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{3.15}$$

Definition 3.1 *Suppose that H(q,p) is a smooth function of its arguments for q and* $p \in \mathbb{R}^n$. *Then the dynamical system (3.14), (3.15) (i = 1,2,...,n) is called a Hamiltonian system and H is the Hamiltonian function (or just the Hamiltonian) of the system. Equations (3.14) and (3.15) called Hamiltons equations.*

In mechanics, the vector q represents the generalized coordinates of the components of the system (positions, angles, etc.), while p is a set of generalized momenta.

Note that for our considered mechanical system $H \equiv T + V$ and thus the Hamiltonian represents the total energy present and the Hamiltonian function is a constant of the motion i.e the Hamiltonian is an invariant of a first integral:

$$\begin{aligned} \frac{dH}{dt} &= \sum_{i=1}^{n} \frac{\partial H}{\partial q_i}\dot{q}_i + \frac{\partial H}{\partial p_i}\dot{p}_i \\ &= \sum_{i=1}^{n} \frac{\partial H}{\partial q_i}\frac{\partial H}{\partial p_i} + \frac{\partial H}{\partial p_i}(-\frac{\partial H}{\partial q_i}) = 0 \end{aligned} \tag{3.16}$$

More generally if a system of ordinary differential equation is defined in terms of $u \in \mathcal{R}^{2d}$ where $u = (q, p)^T$ with $q, p \in \mathcal{R}^d$ such that

$$\dot{u} = f(u) \tag{3.17}$$

Then this system is canonically Hamiltonian if

$$f(u) = J\nabla H \tag{3.18}$$

where $H = H(q, p)$ is the Hamiltonian function and ∇ is the operator

$$(\frac{\partial}{\partial q_1}, \frac{\partial}{\partial q_2}, ..., \frac{\partial}{\partial q_d}, \frac{\partial}{\partial p_1}, \frac{\partial}{\partial p_2}, ..., \frac{\partial}{\partial p_d}) \,, \tag{3.19}$$

and J is the skew symmetric matrix

$$J = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix} \tag{3.20}$$

Here I_d is the identity matrix of dimension d.

In this case f is called a Hamiltonian vector field.

Example 3.1 *A harmonic oscillator is a mass-spring system with potential energy* $\frac{1}{2}kq^2$*, where* q *is the displacement of the spring from equilibrium. For simple systems like this one, in which the potential energy simply depends on the position, the Hamiltonian is just the total energy:*

$$H(q,p) = \frac{1}{2}kq^2 + \frac{p^2}{2m}, \tag{3.21}$$

where k *and* m *are positive constants and* p *is the momentum. Because* H *is a constant, the orbits are just the family of ellipses,*

$$\frac{1}{2}kq^2 + \frac{p^2}{2m} = E \tag{3.22}$$

The value of E *is fixed by the initial conditions. Different values of* E *correspond to ellipses of different size. If we are interested in the equations of motion, we can recover them from Hamiltons equations:*

$$\dot{q} = \frac{\partial H}{\partial p} = p/m \tag{3.23}$$

$$\dot{p} = -\frac{\partial H}{\partial q} = -kq \tag{3.24}$$

3.4.2. Divergence-Free Vector Fields

Another category of vector field with interesting dynamical features are those with zero divergence.

Let $f = f(y), f : \mathcal{R}^d \to \mathcal{R}^d$ be a vector field. Recall that the divergence of f is

$$divf = \frac{\partial}{\partial y_1} f_1 + \frac{\partial}{\partial y_2} f_2 + ... + \frac{\partial}{\partial y_d} f_d \tag{3.25}$$

It happens in certain situations that $divf \equiv 0$. As an illustration, the vector field of the system

$$\frac{dx}{dt} = h_1(y) \tag{3.26}$$
$$\frac{dy}{dt} = h_2(x) \tag{3.27}$$

A very important special case of divergence-free vector fields are those associated to Hamiltonian systems, since, from (3.14) and (3.15) we find

$$divf = \frac{\partial}{\partial q_1}\frac{\partial H}{\partial p_1} + \frac{\partial}{\partial q_2}\frac{\partial H}{\partial p_2} + ... + \frac{\partial}{\partial q_k}\frac{\partial H}{\partial p_k} - \frac{\partial}{\partial p_1}\frac{\partial H}{\partial q_1} - \frac{\partial}{\partial p_2}\frac{\partial H}{\partial q_2} - ... - \frac{\partial}{\partial p_k}\frac{\partial H}{\partial q_k} \tag{3.28}$$

which vanishes due to equality of mixed partial derivatives.

The remarkable feature of divergence-free vector fields is that the flow maps associated to these vector fields are volume preserving.

3.4.3. Volume-Preserving Flows and Liouvilles Theorem

Recall the change of variables theorem tells us that, if we are given a map $\varphi : \mathcal{R}^d \to \mathcal{R}^d$, and a suitable domain $V \subset \mathcal{R}^d$, then

$$volV = \int_V dx, \quad vol(\varphi(v)) = \int_V \left|det\frac{\partial \varphi}{\partial x}\right| dx = \int_V |detM| dx \tag{3.29}$$

where $M = \varphi'$ is the Jacobian of φ.It follows that the map φ preserves volume provided $|detM| = 1$.We would like to examine the Jacobian determinant of the flow map of a system. The flow map itself satisfies

$$\frac{d}{dt}\varphi_t(y) = f(\varphi_t(y)) \tag{3.30}$$

On each side of this equation, we have a vector valued function of y and t; compute the Jacobian matrix of each side, and swap the order of differentiation with respect to t and y:

$$\frac{d}{dt}\varphi_t'(y) = f'(\varphi_t(y))\varphi_t'(y) \tag{3.31}$$

Or $dM/dt = f'(\varphi_t(y))M$. Assuming M is invertible, multiply on the right on both sides by M^{-1}. Compute the trace of each side:

$$tr(\dot{M}M^{-1}) = tr[f'(\varphi_t(y))] \tag{3.32}$$

It is clear to show that $trf' = divf$. *Jacobis* formula for the derivative of a determinant gives

$$tr(\dot{M}M^{-1}) = \frac{\frac{d}{dt}detM}{detM} \tag{3.33}$$

Since $M(0) = \varphi_0'(y) = I$, it follows that

$$det\varphi_t'(y) \equiv 1 \tag{3.34}$$

Thus we have proved the following theorem:

Theorem 3.1 ***(Liouvilles Theorem)****Let a vector field f be divergence free. Then φ_t is a volume preserving map (for all t).*

In particular, all Hamiltonian flow maps preserve volume in phase space. This is a sort of (qualitative) invariant property.

3.4.4. Volume Preserving Numerical Methods

We now ask if there are numerical methods that preserve volume in phase space, i.e. mimicking the corresponding property for the flow map.

The obvious requirement for such a numerical method Φ_h is that

$$divf = 0 \Rightarrow det(\Phi_h') = 1. \tag{3.35}$$

Let us start with Eulers method, $y_{n+1} = y_n + hf(y_n)$. The Jacobian matrix of the flow

$$\Phi_h' = I + hf'(y_n) \tag{3.36}$$

which only has unit determinant in extraordinary situations. For example, the determinant is one for Eulers method applied to the following example:

$$\frac{dx}{dt} = 0 \tag{3.37}$$
$$\frac{du}{dt} = f(x) \tag{3.38}$$

However, it is not one when Eulers method is applied to the harmonic oscillator:

$$\frac{dx}{dt} = u \tag{3.39}$$
$$\frac{du}{dt} = -x \tag{3.40}$$

On the other hand, there are certain methods that do conserve volume, sometimes under special conditions.

3.4.5. Symplectic Integrators

A firs property of Hamiltonian systems, already mentioned in section (3.4.1) is that the Hamiltonian $H(q,p)$ is a first integral of the system (3.11) and (3.12). In this section we shall study another important property-the *symplecticity* of its flow.

The basic objects to be studied are two-dimensional parallelograms lying in $\mathbb{R}^{2d}$. We suppose the parallelogram to be spanned by two vectors

$$\xi = \begin{pmatrix} \xi^q \\ \xi^p \end{pmatrix}, \qquad \eta = \begin{pmatrix} \eta^q \\ \eta^p \end{pmatrix} \tag{3.41}$$

in the (p,q) space $(\xi^q, \xi^p, \eta^q, \eta^p$ are in $\mathbb{R}^d)$ as $P = \{t\xi + s\eta \,|\, 0 \le t \le 1, 0 \le s \le 1\}$. In the case d=1 we consider the *oriented area*

$$Area(P) = det \begin{pmatrix} \xi^q & \eta^q \\ \xi^p & \eta^p \end{pmatrix} = \xi^q\eta^p - \xi^p\eta^q \tag{3.42}$$

In higher dimensions, we replace this by the sum of the oriented areas of the projections of P onto the coordinate planes (p_i, q_i), i.e., by

$$\omega(\xi,\eta) := \sum_{i=1}^{d} det \begin{pmatrix} \xi_i^q & \eta_i^q \\ \xi_i^p & \eta_i^p \end{pmatrix} = \sum_{i=1}^{d} (\xi_i^q \eta_i^p - \xi_i^p \eta_i^q). \tag{3.43}$$

This defines a bilinear map acting on vectors of $\mathbb{R}^{2d}$, which will play a central role for Hamiltonian system. In matrix notation, this map has the form

$$\omega(\xi,\eta) = \xi^T J \eta \qquad \text{with} \qquad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

where I is the identity matrix of dimension d.

Definition 3.2 *A linear mapping $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called symplectic if*

$$A^T J A = J \tag{3.44}$$

or, equivalently, if $\omega(A\xi, A\eta) = \omega(\xi,\eta)$ for all $\xi, \eta \in \mathbb{R}^{2d}$.

We can find it

$$\begin{aligned} \omega(A\xi, A\eta) = (A\xi)^T J (A\eta) &= \xi^T \underbrace{A^T J A}_{J} \eta \\ &= \xi^T J \eta = \omega(\xi,\eta) \end{aligned} \tag{3.45}$$

Definition 3.3 *A differentiable map $g : U \to \mathbb{R}^{2d}$ (where $U \subset \mathbb{R}^{2d}$ is an open set) is called symplectic if the Jacobian matrix $g'(q,p)$ is everywhere symplectic, i.e., if*

$$g'(q,p)^T J g'(q,p) = J \quad \text{or} \quad \omega(g'(q,p)\xi, g'(q,p)\eta) = \omega(\xi,\eta). \tag{3.46}$$

Lemma 3.1 *If ψ and φ are symplectic maps then $\psi \circ \varphi$ is symplectic.*

Proof: *Since* ψ *is symplectic*

$$(\psi')^T J\psi' = J, \qquad \text{similarly} \qquad (\varphi')^T J\varphi' = J$$

$$\left[(\psi o\varphi)'\right]^T J(\psi o\varphi)' = (\psi' o\varphi')^T J(\psi' o\varphi') = (\varphi')^T o(\psi')^T J\psi' o\varphi' = J \tag{3.47}$$

Theorem 3.2 *(Poincaré 1899). Let* $H(q,p)$ *be a twice continuously differentiable function on* $U \subset \mathbb{R}^{2d}$*. Then, for each fixed* t*, the flow* φ_t *is a symplectic transformation wherever it is defined.*

Proof: Let φ_t be flow of the Hamiltonian system. φ_t' is a Jacobian matrix of the flow, then φ_t' satisfies the variational equation i.e.

$$\frac{d}{dt}\varphi_t' = J^{-1}H''\varphi_t' \qquad \text{where} \quad H'' = \begin{pmatrix} H_{pp} & H_{pq} \\ H_{qp} & H_{qq} \end{pmatrix} \quad \text{is symmetric.}$$

Hence

$$\frac{d}{dt}(\varphi_t'^T J\varphi_t') = [J^{-1}H''\varphi_t']^T J\varphi_t' + \varphi_t'^T \underbrace{JJ^{-1}}_{I} H''\varphi_t' \tag{3.48}$$

$$\frac{d}{dt}(\varphi_t'^T J\varphi_t') = \varphi_t'^T H''^T (J^{-1})^T J\varphi_t' + \varphi_t'^T H''\varphi_t' \tag{3.49}$$

Now, we will use $(H'')^T = H''$ and $(J^{-1})^T J = -I$, let us prove it;
$J^T = -J \Rightarrow \quad [(J^{-1})^T J]^T = J^T \cdot J^{-1} = -J \cdot J^{-1} = -I$
then we finally find $(J^{-1})^T J = -I$. We put $(J^{-1})^T J = -I$ in the last equation;

$$\frac{d}{dt}(\varphi_t'^T J\varphi_t') = -\varphi_t'^T H''\varphi_t' + \varphi_t'^T H''\varphi_t' = 0 \tag{3.50}$$

Since $\frac{d}{dt}(\varphi_t'^T J\varphi_t') = 0$ then $\varphi_t'^T J\varphi_t' = \mathbf{C}$. When $t = 0$, we have $\varphi_t'(t_0) = I \Rightarrow C = J$

Theorem 3.3 *Let* $f : U \to \mathbb{R}^{2d}$ *be continuously differentiable. Then,* $\dot{y} = f(y)$ *is locally Hamiltonian if and only if its flow* $\varphi_t(y)$ *is symplectic for all* $y \in U$ *and for all sufficiently small* t*.*

Proof: Assume that the flow φ_t is symplectic, and we have to prove the local existence of a function $H(y)$ such that $f(y) = J^{-1}\nabla H(y)$. Using the fact that $\frac{\partial \varphi_t}{\partial y_0}$ is a solution of the variational equation $\dot{\Psi} = f'(\varphi_t(y_0))\Psi$, we obtain

$$\frac{d}{dt}\left(\left(\frac{\partial \varphi_t}{\partial y_0}\right)^T J\left(\frac{\partial \varphi_t}{\partial y_0}\right)\right) = \left(\frac{\partial \varphi_t}{\partial y_0}\right)\left(f'(\varphi_t(y_0))^T J + J f'(\varphi_t(y_0))\right)\left(\frac{\partial \varphi_t}{\partial y_0}\right) = 0. \quad (3.51)$$

Putting $t = 0$, it follows from $J = -J^T$ that $Jf'(y_0)$ is a symmetric matrix for all y_0.

Definition 3.4 *A numerical one-step method is called symplectic if the one-step map $y_1 = \Phi_h(y_0)$ is symplectic whenever it is applied to a smooth Hamiltonian system.If the method is symplectic:*

$$\Phi_h'(y)^T J \Phi_h'(y) = J \quad (3.52)$$

where $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$

Theorem 3.4 *The implicit midpoint rule is symplectic.*

Proof: The second order implicit midpoint rule is:

$$U_{n+1} = U_n + hf\left(\frac{U_n + U_{n+1}}{2}\right) \quad (3.53)$$

Consider the Hamiltonian problem

$$\dot{y} = J^{-1}\nabla H(y) \quad (3.54)$$

$$U_{n+1} = U_n + hJ^{-1}\nabla H\left(\frac{U_n + U_{n+1}}{2}\right) \quad (3.55)$$

$U_{n+1} = \psi_n(U_n)$ and need to show $\psi_n'^T J \psi_n' = J$

$$\psi_n' = \frac{\partial U_{n+1}}{\partial U_n} = I + hJ^{-1}H''\left(\frac{U_n + U_{n+1}}{2}\right)\left(\frac{1}{2}\right)\left(\frac{\partial U_{n+1}}{\partial U_n} + I\right) \quad (3.56)$$

$$\psi_h' = \frac{\partial U_{n+1}}{\partial U_n} = \left(I - \frac{h}{2}J^{-1}H''\right)^{-1}\left(I + \frac{h}{2}J^{-1}H''\right) \quad (3.57)$$

$\psi_n'^T J \psi_n' = J$ means:

$$\left(I+\frac{h}{2}J^{-1}H''\right)J\left(I+\frac{h}{2}J^{-1}H''\right)^T = \left(I-\frac{h}{2}J^{-1}H''\right)J\left(I-\frac{h}{2}J^{-1}H''\right)^T \tag{3.58}$$

By using the equalities

1) $(H'')^T = H''$ (since H is symmetric)

2) $(J^{-1})^T = -J^{-1} = J$

we get

$$\left(I+\frac{h}{2}J^{-1}H''\right)^T = I-\frac{h}{2}H''J^{-1} \tag{3.59}$$

$$\left(I-\frac{h}{2}J^{-1}H''\right)^T = I+\frac{h}{2}H''J^{-1} \tag{3.60}$$

Then

$$\left(IJ+\frac{h}{2}J^{-1}H''J\right)\left(I-\frac{h}{2}H''J^{-1}\right) = \left(IJ-\frac{h}{2}J^{-1}H''J\right)\left(I+\frac{h}{2}H''J^{-1}\right) \tag{3.61}$$

$$\begin{aligned} &J+\frac{h}{2}J^{-1}H''J-\frac{h}{2}JH''J^{-1}-\frac{h^2}{4}J^{-1}H''JH''J^{-1} \\ &= J+\frac{h}{2}JH''J^{-1}-\frac{h}{2}J^{-1}H''J-\frac{h^2}{4}J^{-1}H''JH''J^{-1} \end{aligned} \tag{3.62}$$

And we find

$$\Rightarrow hJH''J^{-1} = hJ^{-1}H''J \tag{3.63}$$

$$J^{-1} = -J \Rightarrow -JH''J = -JH''J \tag{3.64}$$

Theorem 3.5 *The so-called symplectic Euler method*

$$q_{n+1} = q_n + h\frac{\partial H}{\partial p}(q_{n+1}, p_n) \tag{3.65}$$

$$p_{n+1} = p_n - h\frac{\partial H}{\partial q}(q_{n+1}, p_n) \tag{3.66}$$

is a symplectic method of order 1.

Proof:

$$\begin{pmatrix} p \\ q \end{pmatrix}_{n+1} = \phi_h'\left(\begin{pmatrix} p \\ q \end{pmatrix}_n\right) \tag{3.67}$$

$$\phi_h' = \begin{pmatrix} \frac{\partial p_{n+1}}{\partial p_n} & \frac{\partial p_{n+1}}{\partial q_n} \\ \frac{\partial q_{n+1}}{\partial p_n} & \frac{\partial q_{n+1}}{\partial q_n} \end{pmatrix} \Rightarrow \tag{3.68}$$

$$\frac{\partial p_{n+1}}{\partial p_n} = 1 - hH_{qp}\frac{\partial p_{n+1}}{\partial p_n} \tag{3.69}$$

$$\frac{\partial p_{n+1}}{\partial q_n} = -h[H_{qq}\frac{\partial p_{n+1}}{\partial q_n} + H_{qq}] \tag{3.70}$$

$$\frac{\partial q_{n+1}}{\partial p_n} = hH_{pp}\frac{\partial p_{n+1}}{\partial p_n} \tag{3.71}$$

$$\frac{\partial q_{n+1}}{\partial q_n} = 1 + h(H_{pp}\frac{\partial p_{n+1}}{\partial q_n} + H_{pq}) \tag{3.72}$$

$$(I + H_{qp}^T)\frac{\partial p_{n+1}}{\partial p_n} = I \tag{3.73}$$

$$\Rightarrow \begin{pmatrix} I + hH_{qp}^T & 0 \\ -hH_{pp} & I \end{pmatrix} \begin{pmatrix} \frac{\partial p_{n+1}}{\partial p_n} & \frac{\partial p_{n+1}}{\partial q_n} \\ \frac{\partial q_{n+1}}{\partial p_n} & \frac{\partial q_{n+1}}{\partial q_n} \end{pmatrix} = \begin{pmatrix} I & -hH_{qq} \\ 0 & I + hH_{qp} \end{pmatrix} \tag{3.74}$$

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} X & Y \\ Z & U \end{pmatrix} = \begin{pmatrix} I_m & 0 \\ 0 & I_n \end{pmatrix} \tag{3.75}$$

$$\Rightarrow \begin{pmatrix} X & Y \\ Z & U \end{pmatrix} = \begin{pmatrix} A^{-1} & -A^{-1}.0 \\ -IcA & I^{-1} \end{pmatrix} = \begin{pmatrix} A^{-1} & 0 \\ -cA & I \end{pmatrix} \tag{3.76}$$

$$\begin{matrix} A = I + hH_{qp}^T \\ C = -hH_{pp} \end{matrix} \Rightarrow= \begin{pmatrix} (I + hH_{qp}^T)^{-1} & 0 \\ hH_{pp} + h^2 H_{pp}H_{qp}^T & I \end{pmatrix} \tag{3.77}$$

$$\Rightarrow \left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)}\right) = \begin{pmatrix} (I + hH_{qp}^T)^{-1} & 0 \\ hH_{pp} + h^2 H_{pp}H_{qp}^T & I \end{pmatrix} \begin{pmatrix} I & -hH_{qq} \\ 0 & I + hH_{qp} \end{pmatrix} \tag{3.78}$$

$$= \underbrace{\begin{pmatrix} (I + hH_{qp}^T)^{-1} & -h(I + hH_{qp}^T)^{-1}H_{qq} \\ hH_{pp} + h^2 H_{pp}H_{qp}^T & -h^2 H_{pp}H_{qq} - h^3 H_{pp}H_{qp}^T H_{qq} + I + hH_{qp} \end{pmatrix}}_{K} \tag{3.79}$$

$$K^T = \begin{pmatrix} (I + hH_{qp}^T)^{-1} & hH_{pp}(I + hH_{qp}^T) \\ -h(I + hH_{qp}^T)^{-1}H_{qq} & -h^2 H_{pp}H_{qq} - h^3 H_{pp}H_{qp}^T H_{qq} + I + hH_{qp} \end{pmatrix} \tag{3.80}$$

$$K^T J = \begin{pmatrix} -hH_{pp}(I+hH_{qp}^T) & (I+hH_{qp}^T)^{-1} \\ h^2 H_{pp}H_{qq} + h^3 H_{pp}H_{qp}^T H_{qq} - I - hH_{qp} & -h(I+hH_{qp}^T)^{-1}H_{qq} \end{pmatrix} \tag{3.81}$$

$$K^T JK = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} = J \Rightarrow symplectic$$

Example 3.2 *In this example we look for the application of symplectic integrators to the harmonic oscillator as a Hamiltonian system.*
This well studied problem has a separable Hamiltonian of the form

$$H(p,q) = \frac{q^2}{2} + \frac{p^2}{2}, \tag{3.82}$$

and has solutions which are circles in the (q,p) phase space. The associated differential equations are

$$\frac{dq}{dt} = p, \;\; \frac{dp}{dt} = -q. \tag{3.83}$$

Consider now the closed curve (circle)

$$\Gamma \equiv p^2 + q^2 = C^2, \tag{3.84}$$

the action of the solution operator of the differential equation is to map this curve into itself(conserving the area πC^2 of the enclosed region). The standard forward Euler method applied to this system gives the scheme

$$p_{n+1} = p_n - hq_n, \;\; q_{n+1} = q_n + hp_n, \tag{3.85}$$

so that Ψ_h is the operator given by

$$\Psi_h v = \begin{pmatrix} 1 & -h \\ h & 1 \end{pmatrix} v, \qquad with\ det(\Psi_h) = 1 + h^2. \tag{3.86}$$

It is easy to see that in this case,Γ evolves through the action of the discrete map Ψ_h to the new circle given by

$$p_{n+1}^2 + q_{n+1}^2 = C^2(1+h^2) \tag{3.87}$$

and the area enclosed within the discrete evolution of Γ has increased by a factor of $1+h^2$. Periodic orbits are not preserved by the forward Euler method – indeed all such discrete orbits spiral to infinity. Similarly, a discretisation using the backward Euler method leads to trajectories that spiral towards the origin (Budd and Piggott 2000). Consider now the symplectic Euler method applied to this example. This gives rise to the discrete map

$$p_{n+1} = p_n - hq_n,\ q_{n+1} = q_n + h(p_n - hq_n) = (1-h^2)q_n + hp_n \tag{3.88}$$

The discrete evolutionary is then simply matrix

$$\Psi_h \begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} 1 & -h \\ h & 1-h^2 \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix} \tag{3.89}$$

which can easily be checked to be symplectic. For example det(Ψ_h)=1. The circle Γ is now mapped to the ellipse

$$(1-h^2+h^4)p_{n+1}^2 - 2h^3 p_{n+1}q_{n+1} + (1+h^2)q_{n+1}^2 \ = \ C^2 \tag{3.90}$$

which has the same enclosed area. The symplectic Euler map is not symmetric in time st.

$$\psi_h^{-1} \ \neq \ \psi_{-h}. \tag{3.91}$$

Observe that the symmetry of the circle has been destroyed through the application of this mapping.

It is also easy to see that if

$$A = \begin{pmatrix} 1 & -\frac{h}{2} \\ -\frac{h}{2} & 1 \end{pmatrix} \tag{3.92}$$

then

$$\Psi_h^T A \Psi_h = A. \tag{3.93}$$

3.4.6. Partitioned Systems

In this section we consider partitioned systems

$$\dot{y} = f(y,z) \tag{3.94}$$
$$\dot{z} = g(y,z) \tag{3.95}$$

and separable partitioned systems

$$\dot{y} = f(z) \tag{3.96}$$
$$\dot{z} = g(y) \tag{3.97}$$

In particular, we will be interested in canonical Hamiltonian equations, which are generated by a Hamiltonian function $H(y,z)$ such that

$$f(y,z) = H_z(y,z), \quad g(y,z) = H_y(y,z) \tag{3.98}$$

Such system often arise in mechanical systems described by Hamiltonian function

$$H(q,p) = \frac{p^2}{2} + V(q), \tag{3.99}$$

which provides us with the Hamiltonian equations of motion

$$\dot{q} = p \tag{3.100}$$

$$\dot{p} = -V_q(q) \tag{3.101}$$

Here V is the potential energy function. In the following sections we construct the modified vector field corresponding to partitioned Euler method and its adjoint.

3.4.7. Partitioned Euler Method

In this section we use notations

$$\dot{q} = a(q,p) \tag{3.102}$$

$$\dot{p} = b(q,p) \tag{3.103}$$

Where a and b are the functions of q and p. Then the partitioned Euler method can be given as follows

$$q_{n+1} = q_n + ha(q_{n+1}, p_n), \tag{3.104}$$

$$p_{n+1} = p_n + hb(q_{n+1}, p_n). \tag{3.105}$$

We show the calculation of the functions in modified differential equations. Application of partitioned Euler method to the following modified differential equations which is one term truncated gives a method of order 2.

3.4.8. Symplectic Euler Method

If the partitioned Euler method is applied to a smooth Hamiltonian system then it is called symplectic Euler method. For the Hamilton equations

$$\dot{q} = H_p(q,p) \tag{3.106}$$

$$\dot{p} = -H_q(q,p) \tag{3.107}$$

applying the partitioned Euler method to the system (3.106) and (3.107) we obtain symplectic Euler method given as follows

$$q_{n+1} = q_n + hH_p(q_{n+1}, p_n) \tag{3.108}$$

$$p_{n+1} = p_n - hH_q(q_{n+1}, p_n) \tag{3.109}$$

3.4.9. Construction of the 1-term modified differential equations

The modified vector differential equations are

$$\dot{q} = a(q,p) + hc(q,p) = F(q,p), \tag{3.110}$$

$$\dot{p} = b(q,p) + hd(q,p) = G(q,p). \tag{3.111}$$

Our aim is determining the functions c and d. We determine the function c such as given in the following way.
The Taylor expansion of the exact solution of q for a fixed t is

$$q(t+h) = q(t) + h\dot{q}(t) + \frac{h^2}{2!}\ddot{q(t)} + \frac{h^3}{3!}q^{(3)}(t) + ..., \tag{3.112}$$

where

$$\dot{q}(t) = a \tag{3.113}$$

$$\ddot{q}(t) = a_q\dot{q} + a_p\dot{p} = a_q q + a_p b \tag{3.114}$$

$$\begin{aligned} q^{(3)}(t) &= (a_{qq}\dot{q} + a_{qp}\dot{p})a + a_q(a_q\dot{q} + a_p\dot{p}) + (a_{pq}\dot{q} + a_{pp}\dot{p})b + a_p(b_q\dot{q} + b_p\dot{p}) \\ &= 2a_{qp}(a,b) + a_{qq}(a,a) + a_q a_q a + a_q a_p b \\ &+ a_{pp}(b,b) + a_p b_q a + a_p b_p b \end{aligned} \tag{3.115}$$

Applying the partitioned Euler method to the modified differential equations (3.110) and (3.111) we obtain the following

$$q_{n+1} = q_n + hF(q_{n+1}, p_n) \tag{3.116}$$

$$p_{n+1} = p_n + hG(q_{n+1}, p_n) \tag{3.117}$$

At first considering the equation in (3.116) and substituting F into we get

$$q_{n+1} = q_n + h(a(q_{n+1}, p_n) + hc(q_{n+1}, p_n)) \tag{3.118}$$

We expand each function $a(q_{n+1}, p_n)$ and $c(q_{n+1}, p_n)$ using Taylor expansion and substituting (3.118) instead of q_{n+1} ,

$$\begin{aligned} a(q_{n+1}, p_n) &= a(q_n + \underbrace{hF(q_{n+1}, p_n)}_{\Delta}, p_n) \\ &\simeq a + \Delta a_q \\ &\simeq a + hF(q_{n+1}, p_n)a_q \\ &\simeq a + h(a(q_{n+1}, p_n) + hc(q_{n+1}, p_n))a_q \\ &\simeq a + h(a + hc)a_q \\ &\simeq a + haa_p + h^2 ca_q \end{aligned} \tag{3.119}$$

$$\begin{aligned} c(q_{n+1}, p_n) &= c(q_n + hF(q_{n+1}, p_n), p_n) \\ c(q_{n+1}, p_n) &\simeq c \end{aligned} \tag{3.120}$$

Using the equations (3.119) and (3.120) we write q_{n+1} in the following form

$$q_{n+1} = q_n + h(a + haa_q + h^2 ca_q + hc) \tag{3.121}$$

Comparing the terms of (3.121) and (3.112) with respect to the powers of h we get

$$c = \frac{1}{2}(a_p b - a_q a) \tag{3.122}$$

By the same procedure we can obtain the function d given as follows

$$d = \frac{1}{2}(b_p b - b_q a) \tag{3.123}$$

Now we show the calculation of the functions in 2-term modified differential equations. Application of partitioned Euler method to the following modified differential equations gives a method of order 3.

3.4.10. Construction of the 2-term modified differential equations

The modified vector differential equations are

$$\dot{q} = a(q,p) + hc(q,p) + h^2 e(q,p) = F(q,p) \tag{3.124}$$

$$\dot{p} = b(q,p) + hd(q,p) + h^2 f(q,p) = G(q,p) \tag{3.125}$$

As we determined the functions c and d before we have to determine the functions e and f now. Applying partitioned Euler method to the equations (3.124) and (3.125) we obtain the following

$$q_{n+1} = q_n + hF(q_{n+1}, p_n) \tag{3.126}$$

$$p_{n+1} = p_n + hG(q_{n+1}, p_n) \tag{3.127}$$

At first considering the equation in (3.124) and substituting F into we get

$$q_{n+1} = q_n + h[a(q_{n+1}, p_n) + hc(q_{n+1}, p_n) + h^2 e(q_{n+1}, p_n)] \tag{3.128}$$

We expand each function $a(q_{n+1}, p_n)$, $c(q_{n+1}, p_n)$ and $e(q_{n+1}, p_n)$ using Taylor expansion and substituting (3.128) instead of q_{n+1} ,

$$a(q_{n+1}, p_n) \simeq a + haa_q + h^2 aa_q a_q + h^2 ca_q + \frac{h^2}{2}(a,a)a_{qq} \tag{3.129}$$

$$c(q_{n+1}, p_n) \simeq c + \frac{h}{2}(a_{qp}(a,b) + a_p b_q a - a_{qq}(a,a) - a_q a_q a) \tag{3.130}$$

$$\begin{aligned} e(q_{n+1}, p_n) &= e(q_n + hF(q_{n+1}, p_n), p_n) \\ &\simeq e \end{aligned} \tag{3.131}$$

Using the equations (3.129),(3.130) and (3.131) we write q_{n+1} in the following form

$$\begin{aligned} q_{n+1} &= q_n + h[a + h(aa_q + \frac{1}{2}a_p b - \frac{1}{2}a_q a) + h^2(aa_q a_q + \frac{1}{2}a_p a_q b - \frac{1}{2}a_q a_q a \\ &+ \frac{1}{2}(a,a)a_{qq} + \frac{1}{2}a_{qp}(a,b) + \frac{1}{2}a_p b_q a - \frac{1}{2}a_{qq}(a,a) - \frac{1}{2}a_q a_q a + e)] \quad (3.132) \end{aligned}$$

Comparing the terms of (3.128) and (3.112) with respect to the powers of h we get

$$e = \frac{1}{6}(a_{qq}(a,a) - a_{qp}(a,b) + a_{pp}(b,b) + a_q a_q a - 2a_q a_p b - 2a_p b_q a + a_p b_p b) \quad (3.133)$$

By the same procedure we can obtain the function f given as follows

$$f = \frac{1}{6}(b_{qq}(a,a) - b_{qp}(a,b) + b_{pp}(b,b) + b_q a_q a - 2b_q a_p b - 2b_p b_q a + b_p b_p b) \quad (3.134)$$

If the original equations are Hamiltonian ($a = H_p$, $b = -H_q$), then

$$H^{[3]} = H + \frac{h}{2}(a,b) + \frac{h^2}{6}(H_{qq}(a,a) - H_{qp}(a,b) + H_{pp}(b,b)) \quad (3.135)$$

In view of an important property of this method discovered by de Vogelaere (1956) and we call them *symplectic Euler methods* if we apply the method to Hamiltonian systems (Hairer and Stoffer 1997).

3.4.11. Modifying Symplectic Euler Method for Separable Systems

So far the calculations of the coefficient functions for the modified equations are more complex for the systems we have considered. So we choose separable systems after this section since the calculations of the coefficient functions become more easier. For separable systems the coefficient functions can be given as follows

$$\begin{aligned} c &= \frac{1}{2}a_p b, & d &= -\frac{1}{2}b_q a, & (3.136) \\ e &= \frac{1}{6}(a_{pp}(b,b) - 2a_p b_q a), & f &= \frac{1}{6}(b_{qq}(a,a) - 2b_q a_p a). & (3.137) \end{aligned}$$

If the original equations are Hamiltonian, we get

$$H^{[3]} = H + \frac{h}{2}(a,b) + \frac{h^2}{6}(H_{qq}(a,a) + H_{pp}(b,b)) \tag{3.138}$$

In the application chapter the Harmonic Oscillator and Double Well system will be considered since they are both separable systems.

3.4.12. Modifying Symplectic Euler Method for Mechanical System

For method of order 2 (i.e. the modified differential equations (3.110) and (3.111))

$$\dot{q} = p - \frac{h}{2}V_q(q) \tag{3.139}$$

$$\dot{p} = -V_q(q) + \frac{h}{2}V_{qq}(q)p \tag{3.140}$$

so that we get

$$q_{n+1} = q_n + h(p_n - \frac{h}{2}V_q(q_{n+1})) \tag{3.141}$$

$$p_{n+1} = p_n + h(-V_q(q_{n+1}) + \frac{h}{2}V_{qq}(q_{n+1})p_n) \tag{3.142}$$

The first equation is implicit, the second one is explicit.

3.4.13. Modifying Adjoint Partitioned Euler Method

Definition 3.5 *The adjoint method ϕ_h^* of a method ϕ_h is the inverse map of the original method with reversed time step $-h$ i.e.;*

$$\phi_h^* := \phi_{-h}^{-1} \tag{3.143}$$

In other words, $y_1 = \phi_h^*(y_0)$ is implicitly define by $\phi_{-h}(y_1) = y_0$

The adjoint partitioned Euler method can be given as follows

$$q_{n+1} = q_n + ha(q_n, p_{n+1}), \tag{3.144}$$

$$p_{n+1} = p_n + hb(q_n, p_{n+1}). \tag{3.145}$$

Note that this method is related to the partitioned Euler via the change of variables $u \longleftrightarrow v,\ a \longleftrightarrow b$. Using this relationship, we can obtain the modified differential equations for the adjoint partitioned Euler from those for the partitioned Euler.

We get the modified differential equations

$$\dot{q} = a(q,p) + hc^*(q,p) + h^2 e^*(q,p) \tag{3.146}$$

$$\dot{p} = b(q,p) + hd^*(q,p) + h^2 f^*(q,p) \tag{3.147}$$

by the same procedure we have followed in section (3.4.9) and (3.4.10) we can obtain the functions $c^*, d^*, e^* and f^*$ where

$$c^* = \frac{1}{2}(a_q a - a_p b), \tag{3.148}$$

$$d^* = \frac{1}{2}(b_q a - b_p b), \tag{3.149}$$

$$\begin{aligned} e^* &= \frac{1}{6}(a_{qq}(a,a) - a_{qp}(a,b) + a_{pp}(b,b) + a_q a_q a \\ &- 2a_q a_p b - 2a_p b_q a + a_p b_p b), \end{aligned} \tag{3.150}$$

$$\begin{aligned} f^* &= \frac{1}{6}(b_{qq}(a,a) - b_{qp}(a,b) + b_{pp}(b,b) + b_q a_q a \\ &- 2b_q a_p b - 2b_p b_q a + b_p b_p b). \end{aligned} \tag{3.151}$$

Remark 3.1 *Comparing the modified vector fields for partitioned Euler and its adjoint, we find out that*

$$c^* = -c, \qquad d^* = -d, \qquad e^* = e, \qquad f^* = f. \tag{3.152}$$

Lemma 3.2 *If ϕ is a symplectic map then the adjoint map ϕ^* is symplectic.*

Proof: See (Hairer, et al. 2002)

CHAPTER 4

ANALYSIS FOR MODIFYING INTEGRATORS

In this chapter after designing the new numerical method we analyse it in the concept of *order,consistency* and *stability*.

Definition 4.1 ***Consistency and order:*** *Suppose the numerical method is*

$$y_{n+k} = \phi(t_{n+k}; y_n, y_{n+1}, ..., y_{n+k-1}; h). \tag{4.1}$$

The local error of the method is the error committed by one step of the method. That is, it is the difference between the result given by the method, assuming that no error was made in earlier steps, and the exact solution:

$$\delta^h_{n+k} = \phi(t_{n+k}; y(t_n), y(t_{n+1}), ..., y(t_{n+k-1}); h) - y(t_{n+k}). \tag{4.2}$$

The method is said to be consistent if

$$\lim_{h\to 0} \frac{\delta^h_{n+k}}{h} = 0. \tag{4.3}$$

The method has order p if

$$\delta^h_{n+k} = o(h^{p+1}) \text{ as } h \to 0. \tag{4.4}$$

Hence a method is consistent if it has an order greater than 0. Most methods being used in practice attain higher order. Consistency is a necessary condition for convergence, but not sufficient; for a method to be convergent, it must be both consistent and stable.

A related concept is the global error, the error sustained in all the steps one needs to reach a fixed time t. Explicitly, the global error at time t is $y_N - y(t)$ where $N = (t - t_0)/h$.

The global error of a p^{th} order one-step method is $O(h^p)$; in particular, such a method is convergent. This statement is not necessarily true for multi-step methods.

4.1. Order Analysis for Modifying Symplectic Euler Method

We have pretended in the previous chapter that the application of symplectic Euler method to 1-term modified vector differential equation gives a numerical method of order 2. Note that the symlectic Euler is a method of order 1. Modification of the vector field increases the order of the method. We can show the order of the new modifying method to a mechanical system.

Proposition 4.1 *Application of symplectic Euler method to 1-term modified vector differential equation gives a numerical method of order 2.*

Proof: Consider the mechanical system as we mentioned before given in the equations (3.25) and (3.26). The 1-term modified vector differential equations are

$$\dot{q} = p - \frac{h}{2}V_q(q) \tag{4.5}$$

$$\dot{p} = -V_q(q) + \frac{h}{2}V_{qq}p \tag{4.6}$$

applying the symplectic Euler method to these modified system we get

$$q_{n+1} = q_n + h(p_n - \frac{h}{2}V_q(q_{n+1})) \tag{4.7}$$

$$p_{n+1} = p_n + h(-V_q(q_{n+1}) + \frac{h}{2}V_{qq}(q_{n+1})p_n) \tag{4.8}$$

The first equation is implicit and the second one is explicit.
The Taylor expansions of the exact solutions of $q(x)$ and $p(x)$ about $x = t_n$;

$$q(t_n + h) = q(t_n) + h\dot{q}(t_n) + \frac{h^2}{2!}\ddot{q}(t_n) + \frac{h^3}{3!}q^{(3)}(t_n) + ... \tag{4.9}$$

$$p(t_n + h) = p(t_n) + h\dot{p}(t_n) + \frac{h^2}{2!}\ddot{p}(t_n) + \frac{h^3}{3!}p^{(3)}(t_n) + ... \tag{4.10}$$

Substituting the equalities of $\dot{q}, \ddot{q}, q^{(3)}$ and $\dot{p}, \ddot{p}, p^{(3)}$ in the equations (4.10) and (4.11) we get the following equations

$$\begin{aligned} q(t_n+h) &= q(t_n)+hp(t_n)-\frac{h^2}{2}V_q(q(t_n))-\frac{h^3}{6}V_{qq}(q(t_n))p(q(t_n)+... \quad (4.11)\\ p(t_n+h) &= p(t_n)-hV_q(q(t_n))-\frac{h^2}{2}V_{qq}(q(t_n))p(t_n) \\ &+ \frac{h^3}{6}(-V_{qqq}(q(t_n))p^2(t_n)+V_{qq}(q(t_n))V_q(q(t_n)))+... \quad (4.12)\end{aligned}$$

Since we're just addressing the truncation error, which is introduced in a single step, we can assert $q(t_n) = q_n$ and $q(t_n) = q_n$. Hence

$$\begin{aligned} q(t_n+h) &= q_n+hp_n-\frac{h^2}{2}V_q(q_n)-\frac{h^3}{6}V_{qq}(q_n)p_n+O_1(h^4) \quad (4.13)\\ p(t_n+h) &= p_n-hV_q(q_n)-\frac{h^2}{2}V_{qq}(q_n)p_n \\ &+ \frac{h^3}{6}(-V_{qqq}(q_n)p_n^2+V_{qq}(q_n)V_q(q_n))+O_2(h^4) \quad (4.14)\end{aligned}$$

Now we arrange the equations (4.8) and (4.9). First let us take the equation (4.8).Substituting again (4.8) instead of q_{n+1} and using Taylor's expansion we get

$$\begin{aligned} q_{n+1} &= q_n+h(p_n-\frac{h}{2}V_q(q_{n+1})) \\ &= q_n+hp_n-\frac{h^2}{2}V_q(q_{n+1}) \\ &= q_n+hp_n-\frac{h^2}{2}V_q(q_n+\underbrace{hp_n-\frac{h^2}{2}V_q(q_{n+1})}_{\Delta}) \\ &= q_n+hp_n-\frac{h^2}{2}[V_q(q_n)+\Delta V_{qq}(q_n)+...] \\ &= q_n+hp_n-\frac{h^2}{2}V_q(q_n)-\frac{h^2}{2}(hp_n-\frac{h^2}{2}V_q(q_{n+1}))V_{qq}(q_n)+... \\ &= q_n+hp_n-\frac{h^2}{2}V_q(q_n)-\frac{h^3}{2}V_{qq}(q_n)p_n+... \quad (4.15)\end{aligned}$$

Second let us take the equation (4.9).Substituting again (4.8) instead of q_{n+1} and using Taylor's expansion we get

$$
\begin{aligned}
p_{n+1} &= p_n - hV_q(q_{n+1}) + \frac{h^2}{2}V_{qq}(q_{n+1})p_n \\
&= p_n - hV_q(q_n + \underbrace{hp_n - \frac{h^2}{2}V_q(q_{n+1})}_{\Delta}) \\
&+ \frac{h^2}{2}V_{qq}(q_n + \underbrace{hp_n - \frac{h^2}{2}V_q(q_{n+1})}_{\Delta})p_n \\
p_{n+1} &= p_n - hV_q(q_n) - h\Delta V_{qq}(q_n) - h\frac{\Delta^2}{2}V_{qqq}(q_n) \\
&+ \frac{h^2}{2}V_{qq}(q_n)p_n + \frac{h^2}{2}\Delta V_{qqq}(q_n)p_n + ... \\
&= p_n - hV_q(q_n) - \frac{h^2}{2}V_{qq}(q_n)p_n + \frac{h^3}{2}V_q(q_n)V_{qq}(q_n) + ... \qquad (4.16)
\end{aligned}
$$

Now for finding the errors we subtract the equation (4.16) from (4.14) and (4.17) from (4.15)

$$q(t_n + h) - q_{n+1} = C_1 h^3 \qquad (4.17)$$

$$p(t_n + h) - p_{n+1} = C_2 h^3 \qquad (4.18)$$

Since the truncation error of the method is

$$T_{n+1} = \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} h^3 \qquad (4.19)$$

then the new modifying symplectic Euler method is a method of order 2.

Proposition 4.2 *The 1-term modifying symplectic method is consistent.*

Proof:The consistency of the method is obvious since $\lim_{h\to 0} \frac{T_{n+1}}{h} = 0$.

4.2. Stability Analysis

In this section we give a brief information about stability analysis of scalar and vector valued differential equations.

4.2.1. Stability of a Numerical Method Applied to ODE

To determine whether a numerical method will produce reasonable results with a given value of $h > 0$, we need a notion of stability that is different from zero-stability.There are a wide variety of other forms of stability that have been studied in various contexts. The one that is most basic is absolute stability. This notion is based on the linear test equation,although a study of the absolute stability of a method yields information that is typically directly useful in determining an appropriate time step in nonlinear problems as well.

Theoretical analysis together with numerous numerical experiments has shown that symplectic integrator not only produces improved qualitative numerical behaviors, but also allows for a more accurate long-time scale computation than with general-purpose methods. In the symplectic integration study, a widely recognized fact is that the symplecticity of a numerical integrator has little to do with its step-size.Particularly, for symplectic Runge-Kutta and symplectic partitioned Runge-Kutta methods, their symplecticities are only related to the coefficients(Hairer, et al. 2002).We need to require more stringent conditions on step-sizes in addition to the classical stability considerations in simulations of Hamiltonian flows, even for symplectic integrators. In our work, we make a first step towards such investigation by studying the influence induced by the numerical discretization on the equilibria structure of the underlying Hamiltonian system.

The probably most well known absolute stability is introduced by Dahlquist. Applying the numerical method to the famous test equation

$$y'(t) = \lambda y(t), \quad y(0) = y_0 \, (\neq 0), \quad \lambda \in \mathcal{C}, \quad Re(\lambda) < 0 \tag{4.20}$$

we get the following scheme

$$y_{n+1} = R(z) y_n, \quad n = 0, 1, 2, ..., \ and \ z = \lambda h \tag{4.21}$$

with $R(z)$ the stability function of the method. It is noted that the solution (the analytic solution) to (4.21) asymptotically decays to zero at an exponential rate as $t \to \infty$, and in order for the numerical scheme (4.22) to yield such qualitative behavior without any

restriction on the step size h, we naturally require that

$$|R(z)| \leq 1\ , \quad for \quad any \quad h > 0. \tag{4.22}$$

Methods satisfying (4.23) are called absolutely stable, and this concept has been playing an indispensable role in the numerical field.

Note that there are two parameters h and λ, but only their product $z \equiv h\lambda$ matters. The method is stable whenever $|R(\lambda h)| \leq 1$, and we call this interval as absolute stability interval of the method.

4.2.2. Stability Analysis For Modifying Symplectic Euler Method

In this section we give a brief look to the stability analysis to the new higher order symplectic methods we have constructed in the previous chapter.

So far we have examined stability theory only in the context of a scalar differential equation $y'(t) = f(y(t))$ for a scalar function $y(t)$. In this section we will look at how this stability theory carries over to systems of m differential equations where $y(t) \in \mathbb{R}^m$. For a linear system $y' = Ay$, where A is $m \times m$ matrix, the solution can be written as $y(t) = e^{At}y(0)$ and the behavior is largely governed by the eigenvalues of A. A necessary condition for stability is that $h\lambda$ be in the stability region for each eigenvalue of A. For general nonlinear systems $y' = f(y)$, the theory is more complicated, but a good rule of thumb is that $h\lambda$ should be in the stability region for each eigenvalue of the Jacobian matrix $f'(y)$. This may not be true if the Jacobian is rapidly changing with time, or even for constant coefficient linear problems in some highly nonnormal cases, but most of the time eigenanalysis is surprisingly effective.

Clearly the one-dimensional test equation

$$y'(t) = \lambda y(t),\ \lambda \in \mathbb{C},\ Re(\lambda) < 0,\ t \in [0, \infty) \tag{4.23}$$

is not suitable for the study of absolute stability of partitioned discretization methods as we emphasized in the previous subsection. Since we study mainly on separable systems we have to determine the stability condition of the new proposed methods applied to such systems.

Proposition 4.3 *The new symplectic methods applied to the separable partitioned systems given in (3.26) and (3.27) with test equations*

$$\dot{q} = \alpha p \tag{4.24}$$

$$\dot{p} = \beta q \tag{4.25}$$

that leads to the mapping $y_{n+1} = R(h)y_n$ *said to be stable if* $|Tr(R)| < 2$ *where* $R(h)$ *is the linear stability matrix depending on the coefficients* α ,β *and the time-step h.*

Proof: We have the equation in the form

$$\frac{d}{dt}y = Ay, \tag{4.26}$$

where

$$A = \begin{pmatrix} 0 & \alpha \\ \beta & 0 \end{pmatrix} \tag{4.27}$$

The application of the new method leads to the mapping

$$y_{n+1} = R(h)y_n \tag{4.28}$$

Consider the 2×2 matrix $R(h)$ such that

$$R(h) = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \tag{4.29}$$

A sufficient condition for stability is that the eigenvalues of method are (i) in the unit disc in the complex plane, and (ii) simple (not repeated) if on the unit circle.

Since $R(h)$ is a symplectic map one of its properties is that its determinant is equal to 1. The eigenvalues of the transformation are given by the characteristic equation,

$$\begin{aligned} det\begin{pmatrix} a_{11}-\lambda & a_{12} \\ a_{21} & a_{22}-\lambda \end{pmatrix} &= ((a_{11}-\lambda)(a_{22}-\lambda))-a_{12}a_{21}=0 \\ &= \lambda^2-\underbrace{(a_{11}+a_{22})}_{Tr(R)}\lambda+\underbrace{a_{11}a_{22}-a_{12}a_{21}}_{det(R)=1}=0 \\ &= \lambda^2-Tr(R)\lambda+1=0. \end{aligned} \tag{4.30}$$

The eigenvalues of R are solutions of $\lambda^2-Tr(R)\lambda+1=0$. Following Arnold's treatment of the stability of symplectic maps (Olver 1993), if the two roots λ_1 and λ_2, of this equation are complex conjugates then

$$\lambda=\frac{Tr(R)}{2}\pm i\sqrt{1-\left(\frac{Tr(R)}{2}\right)^2} \tag{4.31}$$

For stability $\lambda<1$, hence $|Tr(R)|<2$ is required. Because the norms of the eigenvalues given in the equation (4.26) are 1 it means that the roots are on the unit circle. For the stability condition the roots can not be multiple if they are on the unit circle.
Since R depends explicitly on the step-size h, it is necessary to take the least positive solution of $|Tr(R)|=2$ with respect to h in the calculation of stability criteria.

4.2.3. Stability Analysis of 1-term Modifying Symplectic Euler Method

The 1 term-modified differential equations of the test equations

$$\dot{q}=\alpha p \tag{4.32}$$

$$\dot{p}=\beta q \tag{4.33}$$

can be found using the functions c and d that we have determined in chapter 3.Such that

$$\dot{q} = \alpha p + \frac{h}{2}\alpha\beta q \tag{4.34}$$

$$\dot{p} = \beta q - \frac{h}{2}\alpha\beta p \tag{4.35}$$

Applying the symplectic Euler method to the equations (4.31) and (4.32) we get the following equations

$$q_{n+1} = q_n + h(\alpha p_n + \frac{h}{2}\alpha\beta q_{n+1}) \tag{4.36}$$

$$p_{n+1} = p_n + h(\beta q_{n+1} - \frac{h}{2}\alpha\beta p_n) \tag{4.37}$$

Proposition 4.4 *The 1-term modifying symplectic Euler method applied to the system (4.31) and (4.32) is stable for* $\left|1 + \frac{1+h^2\alpha\beta}{1-\frac{h^2}{2}\alpha\beta}\right| < 2$

Proof: From the equations (4.33) and (4.34) we can get q_{n+1} and p_{n+1} explicitly. Hence

$$\begin{aligned} q_{n+1} &= \frac{1}{1-\frac{h^2}{2}\alpha\beta} q_n + \frac{h\alpha}{1-\frac{h^2}{2}\alpha\beta} p_n \\ q_{n+1} &= m q_n + n p_n \end{aligned} \tag{4.38}$$

where $m = \frac{1}{1-\frac{h^2}{2}\alpha\beta}$ and $n = \frac{h\alpha}{1-\frac{h^2}{2}\alpha\beta}$.
And

$$\begin{aligned} p_{n+1} &= p_n + h\beta q_n + (1 - h\beta n - \frac{h^2}{2}\alpha\beta) p_n \\ p_{n+1} &= k q_n + l p_n \end{aligned} \tag{4.39}$$

where $k = h\beta m$ and $l = 1 + h\beta n - \frac{h^2}{2}\alpha\beta$.
The equations (4.35) and (4.36) can be written in the matrix form such as

$$\begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \underbrace{\begin{pmatrix} m & n \\ k & l \end{pmatrix}}_{R} \begin{pmatrix} q_n \\ p_n \end{pmatrix} \tag{4.40}$$

where $q(0) = q_0$ and $p(0) = p_0$

$$\begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = R \begin{pmatrix} q_n \\ p_n \end{pmatrix} \tag{4.41}$$

Here R is the linear map we have mentioned before in proposition (4.3) then the stability condition for 1-term modifying Euler method requires $|Tr(R)| = |m+l| = \left|1 + \frac{1+h^2\alpha\beta}{1-\frac{h^2}{2}\alpha\beta}\right| < 2$.

Example 4.1 *The stability condition for the 1-term modifying symplectic Euler method applied to harmonic oscillation problem is $h \in (0,2)$ for the time-step h.*

The harmonic oscillation problem is just a special kind of separable systems which is known as a linear mechanical system. For the linear mechanical systems we pick $\alpha = 1$. The harmonic oscillation problem is

$$\dot{q} = p \tag{4.42}$$

$$\dot{p} = -q \tag{4.43}$$

According to this system $\alpha = 1$ and $\beta = -1$. After substituting these values in the matrix R given in (4.37)we get the following matrix.

$$R = \begin{pmatrix} \frac{1}{1+\frac{h^2}{2}} & \frac{h}{1+\frac{h^2}{2}} \\ \frac{-h}{1+\frac{h^2}{2}} & 1 - \frac{h^2}{1+\frac{h^2}{2}} + \frac{h^2}{2} \end{pmatrix} \tag{4.44}$$

For the matrix R given in (4.41) $|Tr(R)| = \frac{8+h^4}{2(2+h^2)}$ and hence the stability condition is $h \in (0,2)$ for the time-step h.

By the same way we can obtain the stability conditions for other numerical methods applied to different systems.

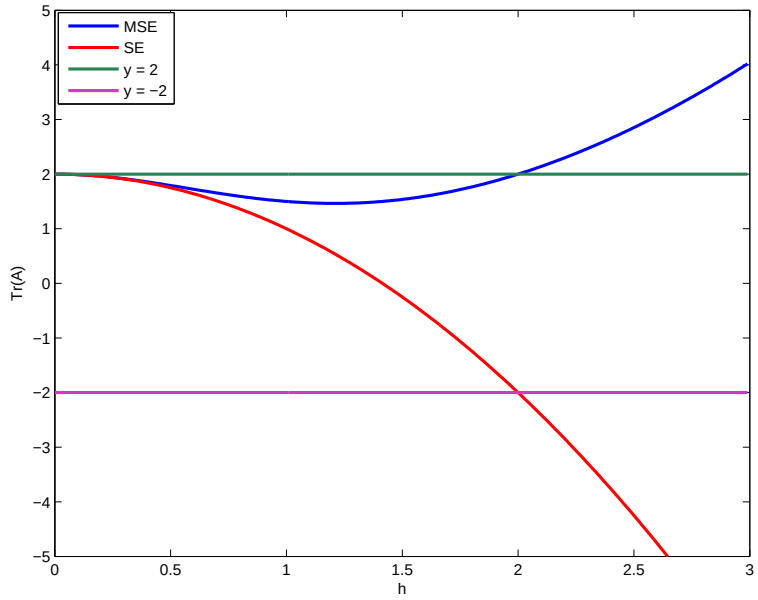

Figure 4.1. Stability Region for the methods MSE and SE

The above figure(4.1) illustrates the stability region for the symplectic Euler method (SE) and 1-term modifying symplectic Euler method (MSE) applied for the Harmonic Oscillation problem. The stability region for the symplectic euler method can be found by the same way. The trace of the matrix A for the symplectic Euler method is $|Tr(R)| = 2 - h^2$. The stability regions are same for two methods.

CHAPTER 5

APPLICATION OF MODIFYING INTEGRATORS

5.1. Applications to Harmonic Oscillator System

In this section we determine the modified differential equations based on the midpoint method and symplectic Euler method for the linear Hamiltonian system which is called Harmonic Oscillator system and illustrate the trajectory of motion (phase space) and the errors in Hamiltonian $|H(q,p) - H(q_0,p_0)|$. The Hamiltonian of this system can be given as

$$H(q,p) = \frac{1}{2}p^2 + \frac{1}{2}q^2 \tag{5.1}$$

so that the equations of motion become

$$\dot{q} = H_p(q,p) = p \tag{5.2}$$

$$\dot{p} = H_q(q,p) = -q \tag{5.3}$$

5.1.1. Modified Equations Based on Midpoint Rule

Let

$$\dot{q} = p = g_1(q,p) \tag{5.4}$$

$$\dot{p} = -q = g_2(q,p) \tag{5.5}$$

The coefficient functions f_j for $j = 2,3,4,5$ of the modified equation can be found by the equations(3.7),(3.8),(3.9) and (3.10). Hence the even indices of the coefficient functions f are zero such that $f_2 = 0$ and $f_4 = 0$.
Now we have to determine the functions f_3 and f_5.

$$f_3 = \frac{1}{12}(-f'f'f + \frac{1}{2}f''(f,f)) \tag{5.6}$$

In equations (5.6) f' is the Jacobian of f. Hence

$$f' = \begin{pmatrix} \frac{\partial g_1}{\partial q} & \frac{\partial g_1}{\partial p} \\ \frac{\partial g_2}{\partial q} & \frac{\partial g_2}{\partial p} \end{pmatrix} \tag{5.7}$$

We have to evaluate the functions $f'f'f$ and $f''(f,f)$ given in equation (5.7)

$$f'f'f = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} p \\ -q \end{pmatrix} = \begin{pmatrix} -p \\ q \end{pmatrix} \tag{5.8}$$

and

$$f''(f,f) = 0 \tag{5.9}$$

Using the equations (5.8) and (5.9) the 2-term modified equation of the harmonic oscillator system can be written as follows

$$f_h^{[3]}(q,p) = \begin{pmatrix} p \\ -q \end{pmatrix} + \frac{h^2}{12} \begin{pmatrix} p \\ -q \end{pmatrix} \tag{5.10}$$

By the same procedure we can evaluate the 4-term modified equation where

$$\begin{aligned} f_5 &= \frac{h^4}{120}(f'f'f'f'f - f''(f,f'f'f) + \frac{1}{2}f''(f'f,f'f)) \\ &+ \frac{h^4}{120}(-\frac{1}{2}f'f'f''(f,f) + f'f''(f,f'f) + \frac{1}{2}f''(f,f''(f,f)) - \frac{1}{2}f^{(3)}(f,f,f'f)) \\ &+ \frac{h^4}{80}(-\frac{1}{6}f'f^{(3)}(f,f,f) + \frac{1}{24}f^{(4)}(f,f,f,f)). \end{aligned} \tag{5.11}$$

given as follows

$$f_h^{[5]}(q,p) = \begin{pmatrix} p \\ -q \end{pmatrix} + \frac{h^2}{12} \begin{pmatrix} p \\ -q \end{pmatrix} + \frac{h^4}{120} \begin{pmatrix} p \\ -q \end{pmatrix} \tag{5.12}$$

Application of the midpoint rule to the modified equation (5.10) and (5.12) gives a method of order 4 and 6 respectively.

5.1.2. Modified Equations Based on Symplectic Euler Method

Let

$$\dot{q} = p = a(q,p) \tag{5.13}$$

$$\dot{q} = -q = b(q,p) \tag{5.14}$$

The coefficient functions $c(q,p)$,$d(q,p)$,$e(q,p)$ and $f(q,p)$ of the modified equation can be found using the equations (3.136) and(3.137). We obtain the modified differential equations of the system (5.13) and (5.14) in the form

$$\dot{y} = f_h^{[i]}(y), \quad for \quad i = 2,3 \quad where \quad y = (q,p) \tag{5.15}$$

where

$$f_h^{[2]}(q,p) = \begin{pmatrix} p \\ -q \end{pmatrix} + \frac{h}{2}\begin{pmatrix} -q \\ p \end{pmatrix} \tag{5.16}$$

$$f_h^{[3]}(q,p) = \begin{pmatrix} p \\ -q \end{pmatrix} + \frac{h}{2}\begin{pmatrix} -q \\ p \end{pmatrix} + \frac{h^2}{3}\begin{pmatrix} p \\ -q \end{pmatrix} \tag{5.17}$$

5.1.3. Numerical Implementation for Harmonic Oscillation

In this section numerical methods are applied to the Harmonic Oscillator system. We apply symplectic Euler method (SE) (order1), Stmer-Verlet method (SVM)(order2), Lobatto method (order2) and Midpoint rule (MR) (order2) to the system (5.13) and (5.14) and symlectic Euler method to the equation (5.15). For $i = 2$ and $i = 3$ application of symplectic Euler method gives a method of order 2 and 3 respectively.

The Figures (5.1, 5.2, 5.3, 5.4, 5.5, 5.6) illustrates the trajectory of motion and errors in Hamiltonian (conservation of energy) obtained by symplectic Euler (SE), 1-term modifying symplectic Euler (MSE2), 1-term modifying adjoint symplectic Euler

(AMSE2),Strmer-Verlet (SVM), Lobatto and Midpoint rule (MR) methods respectively. Since all of these methods are symplectic geometric integrators the shape of the trajectory preserved by both these methods. The 1-term modifying symplectic Euler method conserves the energy better than the other methods except midpoint rule.

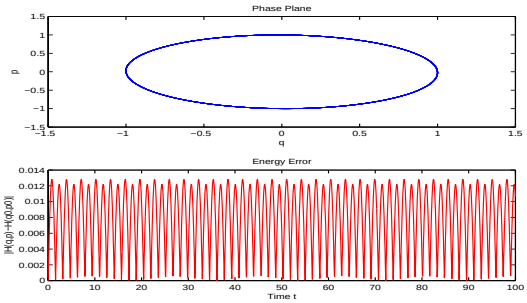

Figure 5.1. Trajectory of motion and error in Hamiltonian by SE

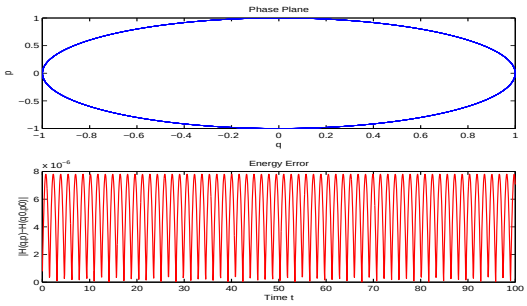

Figure 5.2. Trajectory of motion and error in Hamiltonian by MSE2

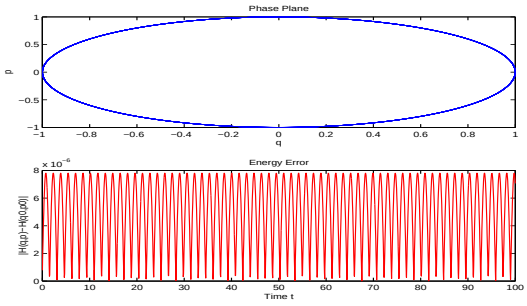

Figure 5.3. Trajectory of motion and error in Hamiltonian by AMSE2

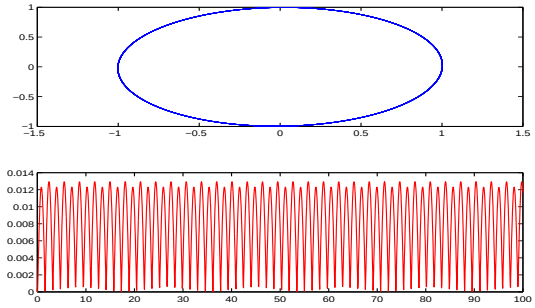

Figure 5.4. Trajectory of motion and error in Hamiltonian by SVM

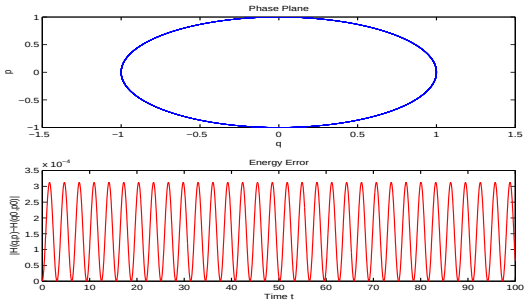

Figure 5.5. Trajectory of motion and error in Hamiltonian by Lobatto Method

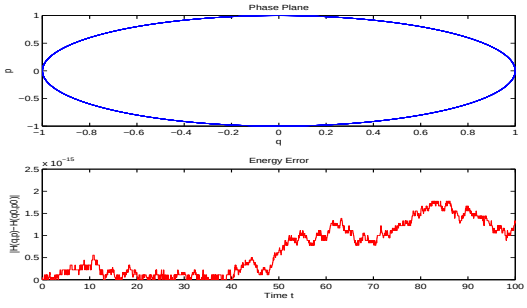

Figure 5.6. Trajectory of motion and error in Hamiltonian by MR

5.2. Applications to Harmonic Double Well System

In this section we determine the modified differential equations based on the midpoint method and symplectic Euler method for the nonlinear Hamiltonian system which is called Double Well system and illustrate the trajectory of motion (phase space) and the errors in Hamiltonian $|H(q,p)-H(q_0,p_0)|$. The Hamiltonian of this system can be given as

$$H(q,p)=\frac{1}{2}p^2+\frac{1}{2}(q^2-1).^2 \tag{5.18}$$

so that the equations of motion become

$$\dot{q} = H_p(q,p)=p=a(q,p) \tag{5.19}$$

$$\dot{p} = H_q(q,p)=-2q(q^2-1)=b(q,p) \tag{5.20}$$

In this section we derive only the modified differential equations of the system (5.19) and (5.20) based on symplectic Euler method. The coefficient functions $c(q,p), d(q,p)$, of the modified equation can be found using the equations (3.122) and(3.123). We obtain the modified differential equations of the system (5.19) and (5.20) in the form

$$\dot{y}=f_h^{[i]}(y), \quad for \quad i=2 \quad where \quad y=(q,p) \tag{5.21}$$

where

$$f_h^{[2]}(q,p)=\begin{pmatrix} p \\ -2q(q^2-1) \end{pmatrix}+h\begin{pmatrix} -q(q^2-1) \\ (3q^2-1)p \end{pmatrix} \tag{5.22}$$

5.2.1. Numerical Implementation for Double Well

In this section numerical methods are applied to the Double Well system. We apply symplectic Euler method (SE)(order1), Stmer-Verlet method (SVM) (order2), Lobatto method (order2) and Midpoint rule (MR) (order2) to the system (5.19) and (5.20) and symlectic Euler method to the equation (5.22). For $i=2$ application of symplectic Euler method gives a method of order 2 (MSE2).

The Figures (5.7, 5.8, 5.9, 5.10, 5.11, 5.12, 5.13) illustrates the trajectory of motion and errors in Hamiltonian (conservation of energy) obtained by symplectic Euler (SE), 1-term modifying symplectic Euler (MSE2), 1-term modifying adjoint symplectic Euler (AMSE2), Strmer-Verlet (SVM), Lobatto , Midpoint rule methods (MR) and ODE-45 respectively. Since all of these methods are symplectic geometric integrators the shape of the trajectory preserved by both these methods. The 1-term modifying symplectic Euler method conserves the energy better than symplectic Euler method.

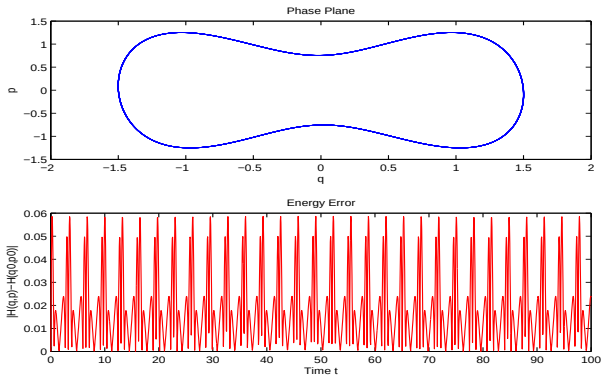

Figure 5.7. Trajectory of motion and error in Hamiltonian by SE

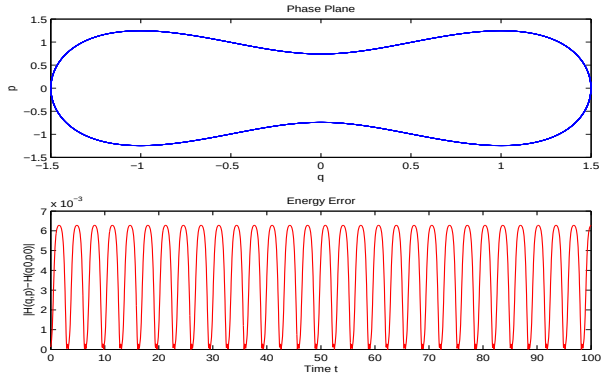

Figure 5.8. Trajectory of motion and error in Hamiltonian by MSE2

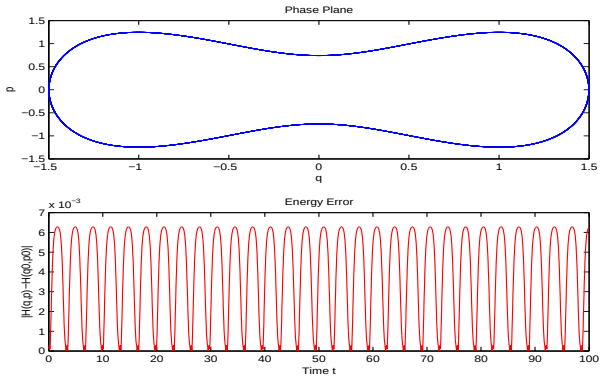

Figure 5.9. Trajectory of motion and error in Hamiltonian by AMSE2

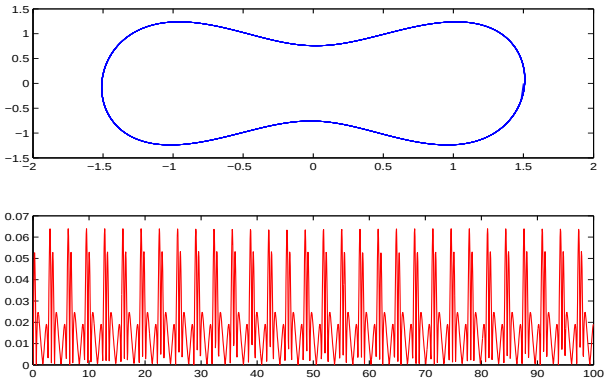

Figure 5.10. Trajectory of motion and error in Hamiltonian by SVM

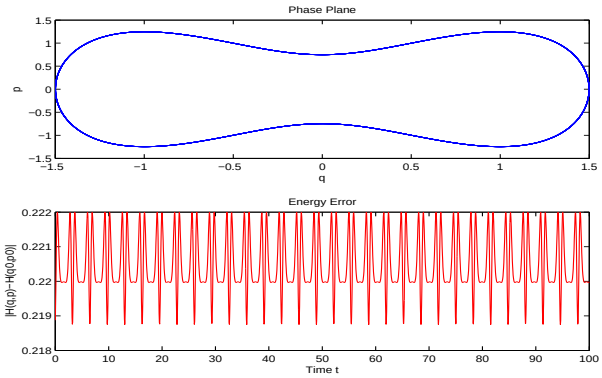

Figure 5.11. Trajectory of motion and error in Hamiltonian by Lobatto Method

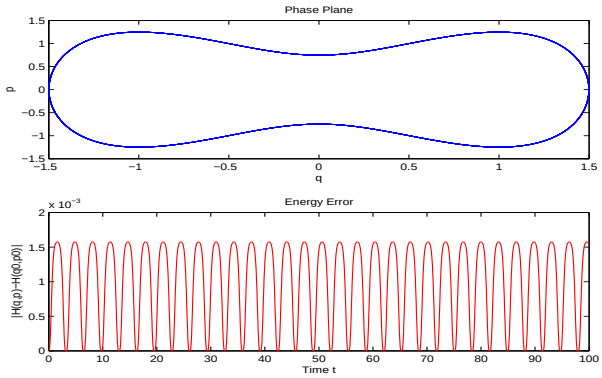

Figure 5.12. Trajectory of motion and error in Hamiltonian by Midpoint Rule

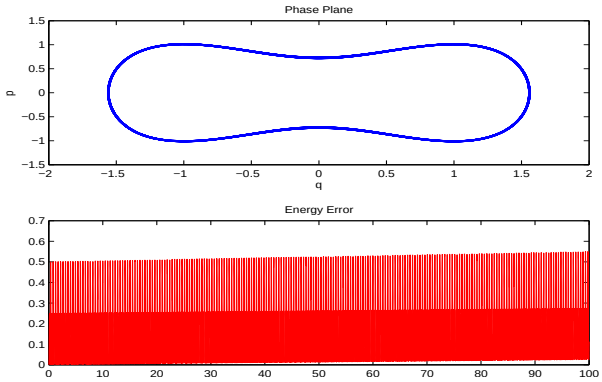

Figure 5.13. Trajectory of motion and error in Hamiltonian by ODE45

CHAPTER 6

SUMMARY AND CONCLUSION

In this thesis new higher order symplectic methods using the idea of modified vector fields are constructed. The stability and consistency analysis are studied and the proposed new methods are applied to some seprable Hamiltonian systems such as Harmonic Oscillation and Double Well problems as a numerical test problem and the resuls obtained from these new methods are compared with classical methods. All algorithms of the methods were written in MATLAB.

As a conclusion, the following results are obtained:

• Modified symplectic Euler method of order 2 and order 3 (MSE2 and MSE3) give better performance than Strmer-Verlet Method (SVM) and ODE-45.

• Order of symplectic Euler method is increased to 2 and 3.

• Stability regions do not change for symplectic Euler and modified symplectic Euler methods.

• Modified symplectic Euler method is a combination of implicit and explicit (IMEX methods).

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APPENDIX A

MATLAB CODES

A.1. Methods Applied to Harmonic Oscillation Problem

A.1.1. Stability Function

```
for i=1:300
 x(i)=(i-1)*0.01 ;
 y(i)=(8+(x(i).^4))/(4+2*(x(i).^2));
 z(i)=(2-(x(i).^2))
 w(i)=2;
 v(i)=-2;
end
plot(x,y);
hold on;plot(x,z,'r');plot(x,w,'g');plot(x,v,'m');
xlabel('h');
ylabel('Tr(A)');
axis([0, 3, -5, 5]);
legend('MSE','SE','y=2','y=-2');
```

A.1.2. Symplectic Euler Method

```
h = 0.05 ;
q(1)  = 1 ;
p(1)  = 0 ;
t=0:h:100;
n=100/h+1;
 for i=1:n
      ye(i)=cos(t(i));
  end
```

```
for i=1:n
    H(i)=.5*((q(i).^2)+(p(i).^2));
    q(i+1)=q(i)+h*p(i);
    p(i+1)=p(i)-h*q(i+1);
    er(i)=ye(i)-q(i);
    e(i)=abs(H(i)-H(1));
end
subplot(211);plot(q,p);
title('Phase Plane');
xlabel('q');ylabel('p');
subplot(212);plot(t,e,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
```

A.1.3. Modifying Symplectic Euler Method of Order 2

```
h = 0.05 ;
x0  = 1 ;
p0  = 0 ;
x = x0 ;
p = p0 ;
H0 =  (  ( p*p/2 ) +  ( x*x/2 ));
t=0:h:100;
N=100/h+1;

for i=1:N
ye(i)=cos(t(i));
end
  for i = 1:N
 x1 = x ;
 x2 = x1 ;
 for k = 1:N
```

```
 x2 =  x + h * (p-.5*h*x1);
 x1= x2 ;
 end
  p1 =  p + h*(-x1+.5*h*p);
  X(:,i) = x1 ;
  P(:,i) = p1;
  x = x1;
  p = p1;
  er(i)=ye(i)-x;
 H(i)  =  (  ( p'*p/2 ) + ( x'*x/2 ) ) ;
 error_H(i)  =abs(H(i)   - H0)  ;
  end
subplot(211);plot(X,P);
title('Phase Plane');
xlabel('q');ylabel('p');
subplot(212);plot(error_H,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
```

A.1.4. Adjoint Modifying Symplectic Euler Method of Order 2

```
h = 0.05 ;
x0  = 1 ;
p0  = 0 ;
x = x0 ;
p = p0 ;
H0 =  (  ( p*p/2 ) +  ( x*x/2 ));
t=0:h:100;
N=100/h+1;
for i=1:N
ye(i)=cos(t(i));
end
```

```
  for i = 1:N
p1 = p;
p2 = p1;
for k = 1:N
    p2=p-h*(x+.5*h*p1);
    p1=p2;
end
x1=x+h*(p1+.5*h*x);
X(:,i) = x1 ;
P(:,i) = p1;
x = x1;
p = p1;
 er(i)=ye(i)-x;
 H(i)  =  (  ( p'*p/2 ) + ( x'*x/2 ) ) ;
 error_H(i)  =abs(H(i)   - H0)  ;
  end
subplot(211);plot(X,P);
title('Phase Plane');
xlabel('q');ylabel('p');
subplot(212);plot(t,error_H,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
```

A.1.5. Strmer-Verlet Method

```
h = 0.05 ;
q1(1)  = 1 ;
p1(1)  = 0 ;
q2(1)  = 1 ;
p2(1)  = 0 ;
t=0:h:100;
N=100/h+1;
```

```
for i=1:N
     H(i)=.5*((p2(i).^2)+(q2(i).^2));
     er(i)=abs(H(i)-H(1));
 p1(i+1)=p1(i)-h*q1(i);
 q1(i+1)=q1(i)+h*p1(i+1);
 q2(i+1)=q1(i+1)+h*p1(i+1);
  p2(i+1)=p1(i+1)-h*q2(i+1);
end
subplot(211);plot(q2,p2);
subplot(212);plot(t,er,'r');
```

A.1.6. Lobatto Method

```
p0= 1;
q0= 0;
h=.05;
t=0:h:100;
n=100/h+1;
q=q0;
p=p0;
H0= 0.5;
L1p=feval('hpp',q,p);
k2p=feval('hpp',q,p);
for i=1:n
     ye(i)=sin(t(i));
end
for i=1:n
% Calculation of  of L1 implicit
  for j=1:5
      L1=feval('hpp',q, p+h/2*L1p);
       L1p=L1;
  end
```

```
 % Calculation of  of k1 explicit
     k1=feval('hqp',q,p+h/2*L1);
  for j=1:5
 % Calculation of  of k2 implicit
     k2=feval('hqp',q + h/2*(k1+k2p),p+h/2*L1);
      k2p=k2;
  end
 % Calculation of  of L2 explicit
   L2=feval('hpp',q + h/2*(k1+k2),p+h/2*L1);
q1=q+ h/2*(k1+k2);
p1=p+(h/2)*(L1+L2);
  Q(:,i) = q1;
  P(:,i) = p1;
  q= q1;
  p= p1;
  er(i)=ye(i)-q;
e(i)= .5*((p.^2)+(q.^2)) - 0.5;
end
subplot(211);plot(Q,P);
title('Phase Plane');
xlabel('q');ylabel('p');
subplot(212);plot(t,e,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
```

A.1.7. Midpoint Method

```
h = 0.05 ;
x0  = 1 ;
p0  = 0 ;
x = x0 ;
p = p0 ;
```

```
H0 =  (  ( p*p/2 ) +  ( x*x/2 ));
t=0:h:100;
N=100/h+1;
for i=1:N
ye(i)=cos(t(i));
end
for i = 1:N
x1 = x ;
p1 = p;
x2 = x1 ;
p2 = p1;
for k=1:N
p_mid  = (p+p1)/2;
x2 =  x + h * p_mid ;
x_mid  = (x+x1)/2;
p2 =  p - h*x_mid;
x1= x2;
p1 = p2;
end;
X(:,i) = x1 ;
P(:,i) = p1;
x = x1;
p = p1;
er(i)=(ye(i)-x);
H(i)  =  (  ( p*p/2 ) + ( x'*x/2 ) ) ;
error_H(i)  =abs(H(i)   - H0)  ;
end;
subplot(211);plot(X,P);
title('Phase Plane');
xlabel('q');ylabel('p');
subplot(212);plot(t,error_H,'r');
title('Energy Error');
```

```
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
```

A.2. Methods Applied to Double Well Problem

A.2.1. Symplectic Euler Method

```
h = 0.05 ;
q(1)  = 1.5 ;
p(1)  = 0 ;
t=0:h:100;
n=100/h+1;
for i=1:n
H(i) = (  ( p(i)*p(i)/2 ) +  ( (((q(i).^2)-1).^2)/2 ));
q(i+1)=q(i)+h*p(i);
p(i+1)=p(i)-2*h*q(i+1)*((q(i+1).^2)-1);
e(i)=abs(H(i)-H(1));
end
subplot(211);plot(q,p);
title('Phase Plane');
xlabel('q');ylabel('p');
subplot(212);plot(t,e,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
```

A.2.2. Modifying Symplectic Euler Method of Order 2

```
      h = 0.05 ;
x0  = 1.5 ;
p0  = 0 ;
x = x0 ;
p = p0 ;
H0 =  (  ( p*p/2 ) +  ( (((x.^2)-1).^2)/2 ));
```

```
t=0:h:100;
N=100/h+1;
  for i = 1:N
 x1 = x ;
 x2 = x1 ;
 for k = 1:N
 x2 =  x + h * (p-h*x1*(x1.^2-1));
 x1= x2 ;
 end
  p1 =  p + h*(-2*x1*(x1.^2-1)+h*p*((3*x1.^2)-1));
  X(:,i) = x1 ;
  P(:,i) = p1;
  x = x1;
  p = p1;
 H(i)  =  (  ( p*p/2 ) +  ( (((x.^2)-1).^2)/2 ));
 error_H(i)  =abs(H(i)   - H0)  ;
 end;
subplot(211);plot(X,P);
title('Phase Plane');
xlabel('q');ylabel('p');
subplot(212);plot(t,error_H,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
```

A.2.3. Adjoint Modifying Symplectic Euler Method of Order 2

```
      h = 0.05 ;
x0  = 1.5 ;
p0  = 0 ;
x = x0 ;
p = p0 ;
H0 =  (  ( p*p/2 ) +  ( (((x.^2)-1).^2)/2 ));
```

```
t=0:h:100;
N=100/h+1;
  for i = 1:N
p1 = p;
p2 = p1;
for k = 1:N
    p2=p+h*(-2*x*((x.^2)-1)-h*(3*(x.^2)-1)*p1);
    p1=p2;
end
x1=x+h*(p1+h*x*((x.^2)-1));
X(:,i) = x1 ;
P(:,i) = p1;
x = x1;
p = p1;
 H(i) = (  ( p*p/2 ) +  ( (((x.^2)-1).^2)/2 ));
 error_H(i)  =abs(H(i)   - H0)  ;
  end
subplot(211);plot(X,P);
title('Phase Plane');
xlabel('q');ylabel('p');
subplot(212);plot(t,error_H,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
```

A.2.4. Strmer-Verlet Method

```
h = 0.05 ;
q1(1)  = 1.5 ;
p1(1)  = 0 ;
q2(1)  = 1.5 ;
p2(1)  = 0 ;
t=0:h:100;
```

```
N=100/h+1;
for i=1:N
     H(i)=.5*((p2(i).^2)+((q2(i).^2)-1).^2);
     er(i)=abs(H(i)-H(1));
 p1(i+1)=p1(i)-h*(2*q1(i)*(q1(i).^2-1));
 q1(i+1)=q1(i)+h*p1(i+1);
 q2(i+1)=q1(i+1)+h*p1(i+1);
  p2(i+1)=p1(i+1)-h*(2*q2(i+1)*(q2(i+1).^2-1));
end
subplot(211);plot(q2,p2);
subplot(212);plot(t,er,'r');
```

A.2.5. Lobatto Method

```
clear all;
q0= 1.5;
p0= 0;
h=.05;
t=0:h:100;
n=100/h+1;
q=q0;
p=p0;
H0= 1;
L1p=feval('lpp',q,0);
k2p=feval('lpp',q,p);
for i=1:n
     ye(i)=sin(t(i));
end
for i=1:n
% Calculation of  of L1 implicit
  for j=1:5
      L1=feval('lpp',q, p+h/2*L1p);
```

```
      L1p=L1;
  end
 % Calculation of  of k1 explicit
     k1=feval('lqp',q,p+h/2*L1);
  for j=1:5
 % Calculation of  of k2 implicit
     k2=feval('lqp',q + h/2*(k1+k2p),p+h/2*L1);
      k2p=k2;
  end
 % Calculation of  of L2 explicit
   L2=feval('lpp',q + h/2*(k1+k2),p+h/2*L1);
q1=q+ h/2*(k1+k2);
p1=p+(h/2)*(L1+L2);
  Q(:,i) = q1;
  P(:,i) = p1;
  q= q1;
  p= p1;
  er(i)=ye(i)-q;
e(i)= abs(.5*((p.^2)+((q.^2)-1).^2) - 1);
end
subplot(211);plot(Q,P);
title('Phase Plane');
xlabel('q');ylabel('p');
subplot(212);plot(t,e,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
```

A.2.6. Midpoint Method

```
h = 0.05 ;
x0  = 1.5 ;
p0  = 0 ;
```

```
x = x0 ;
p = p0 ;
H0 =  (  ( p*p/2 ) +  ( (((x.^2)-1).^2)/2 ));
t=0:h:100;
N=100/h+1;
for i = 1:N
x1 = x ;
p1 = p;
x2 = x1 ;
p2 = p1;
for k=1:N
p_mid  = (p+p1)/2;
x2 =  x + h * p_mid ;
x_mid  = (x+x1)/2;
p2 =  p - 2*h*x_mid*((x_mid.^2)-1);
x1= x2;
p1 = p2;
end;
X(:,i) = x1 ;
P(:,i) = p1;
x = x1;
p = p1;
H(i)  =  (  ( p*p/2 ) +  ( (((x.^2)-1).^2)/2 ));
error_H(i)  =abs(H(i)   - H0)  ;
end;
subplot(211);plot(X,P);
title('Phase Plane');
xlabel('q');ylabel('p');
subplot(212);plot(t,error_H,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
```

A.2.7. ODE-45

```
       options = odeset('RelTol',1e-4,'AbsTol',[1e-4 1e-4]);
[t,Y] = ode45(@rigid,[0 870],[-1 1.000001 ],options);


h=100/10025;
q0=-1;
p0=1.000001;
q=Y(:,1);
p=Y(:,2);
H0=  0.5* (p0.^2) - 0.5* (q0.^2- 1).^2;
t=0+h:h:100;

for i=1:n
   P(i) = Y(i,2);
   Q(i)= Y(i,1);
   H(i) =   ( P(i).^2 /2 ) + 0.5*(( Q(i).^2 ) -1 ).^2;
   error(i)  =  H(i)   - H0;
end
size(t)
size (error)
subplot(211);plot(q,p);
title('Phase Plane');
xlabel('q');ylabel('p');
subplot(212);plot(t,error,'r');
title('Energy Error');
```