

## Application of Lie transform perturbation method for multidimensional non-Hermitian systems

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**Abstract.** Three-dimensional non-Hermitian systems are investigated using classical perturbation theory based on Lie transformations. Analytic expressions for total energy in terms of action variables are derived. Both real and complex semiclassical eigenvalues are obtained by quantizing the action variables. It was found that semiclassical energy eigenvalues calculated with the classical perturbation theory are in very good agreement with exact energies and for certain non-Hermitian systems second-order classical perturbation theory performed better than the second-order Rayleigh–Schroedinger perturbation theory.

**Keywords.** Classical perturbation theory; non-Hermitian quantum mechanics; Birkhoff normal forms.

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### 1. Introduction

Classical perturbation theory based on Lie transforms has been used to investigate the motion of an artificial satellite [1] and to obtain constants of motion of 2D coupled harmonic oscillator systems [2]. On the other hand, the classical perturbation theory in conjunction with semiclassical quantization techniques has been utilized for determining semiclassical eigenenergies and linking quantum avoided crossing with classical chaos in real Hermitian systems in the past [3,4].

In recent years, quantum as well as classical behaviour of complex non-Hermitian Hamiltonian systems have been of great interest because certain 1D and multidimensional complex non-Hermitian systems possess purely real spectra [5–14]. It was revealed in classical mechanical studies that the classical motion of complex non-Hermitian systems has rich and complicated behaviour compared to that of Hermitian systems. It was also found strange that new kinds of classical trajectories are not PT symmetric although the PT symmetry is not spontaneously broken [15].

Semiclassical investigations of non-Hermitian complex Hamiltonian systems are important from both fundamental and practical points of views. In the first place they may expose important clues hidden in the correspondence between classical and quantum mechanics, specially when classical motion becomes chaotic or PT symmetries of quantum states are spontaneously broken. Secondly, they provide powerful tools for calculating highly excited energy spectra of the multidimensional complex systems. Particularly, when action variables or eigenenergy expressions are available in analytic form, it is possible to have a better understanding of the classical behaviour, the semiclassical quantization and the semiclassical limit.

In this paper we obtain semiclassical eigenenergies of 3D non-Hermitian Hamiltonians as analytic expressions using second-order classical perturbation theory based on Lie transformation. We examine the accuracy of both real and complex energy eigenvalues of these systems when they are PT symmetric and non-pseudo-Hermitian.

The first 3D system of interest is the PT symmetric system

$$H_a = \frac{p_1^2}{2} + \frac{p_2^2}{2} + \frac{p_3^2}{2} + \omega_1^2 x_1^2 + \omega_2^2 x_2^2 + \omega_3^2 x_3^2 + i\lambda x_1 x_2 x_3, \quad (1)$$

where  $\lambda$  is real. The quantum eigenenergy spectra of this system are real and positive [16]. The second system is the 3D version of Henon–Heiles system,

$$H_b = \frac{p_1^2}{2} + \frac{p_2^2}{2} + \frac{p_3^2}{2} + \omega_1^2 x_1^2 + \omega_2^2 x_2^2 + \omega_3^2 x_3^2 + i\lambda(x_1 x_2^2 + \alpha x_1^3) + i\mu(x_2 x_3^2 + \beta x_2^3), \quad (2)$$

where  $\lambda, \mu, \alpha$  and  $\beta$  can be real or complex. When all of them are real, the system is PT symmetric whereas if  $\lambda$  and  $\mu$  are not pure imaginary and  $\alpha$  and  $\beta$  are non-real, the system is neither PT symmetric nor pseudo-Hermitian. In the former case, the system has real and positive eigenvalues whereas for the latter case the system will have complex eigenvalues. First we derive classical Lie canonical transform equations for 3D systems before presenting semiclassical eigenenergy expressions.

## 2. Classical Lie canonical transform

In this section, first we describe the classical perturbation theory based on Lie canonical transformations. Consider the Hamiltonian of the form

$$H = H_0 + \epsilon H_1, \quad (3)$$

where

$$H_0 = \frac{1}{2} [p_1^2 + p_2^2 + \omega_1^2 x_1^2 + \omega_2^2 x_2^2 + \omega_3^2 x_3^2] \quad (4)$$

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and  $H_1(x_1, x_2, x_3)$  makes the above Hamiltonian  $H$  non-separable and non-Hermitian. Hamilton's equation of motion for the above Hamiltonian is

$$\frac{dp_j}{dt} = -\frac{\partial H}{\partial x_j} \quad (5)$$

and

$$\frac{dx_j}{dt} = \frac{\partial H}{\partial p_j} \quad (6)$$

( $j = 1, 2, 3$ )

Now consider the transformation  $(p_j, x_j) \rightarrow (\eta_j, \xi_j)$  given by

$$p_j = \eta_j - \epsilon \frac{\partial S_1}{\partial \xi_j} - \epsilon^2 \frac{\partial S_2}{\partial \xi_j} - \frac{1}{2} \epsilon^2 \left\{ \frac{\partial S_1}{\partial \xi_j}, S_1 \right\} + O(\epsilon^3) \quad (7)$$

and

$$x_j = \xi_j + \epsilon \frac{\partial S_1}{\partial \eta_j} + \epsilon^2 \frac{\partial S_2}{\partial \eta_j} + \frac{1}{2} \epsilon^2 \left\{ \frac{\partial S_1}{\partial \eta_j}, S_1 \right\} + O(\epsilon^3), \quad (8)$$

where  $\{\}$  represents the Poisson bracket (Note that the Poisson bracket used here is defined with respect to conjugate complex variables  $\xi_j$  and  $\eta_j$ . Therefore, the non-standard Poisson bracket defined in [17] does not apply here.) The functions  $S_1, S_2, \dots$  are defined later in terms of the Hamiltonian (for details, see [1,2]). Then the equations of motion becomes

$$\frac{d\eta_j}{dt} = -\frac{\partial H^*}{\partial \xi_j}, \quad (9)$$

$$\frac{d\xi_j}{dt} = \frac{\partial H^*}{\partial \eta_j}, \quad (10)$$

where  $j = 1, 2, 3$  and the new Hamiltonian  $H^*(\eta, \xi) = H(p, x)$ . The purpose for introducing this canonical transformation is, to eliminate, from Hamiltonian  $H^*$ , the parameter  $\tau$  which is introduced in eqs (12) and (13). Now we expand  $H^*$  in a power series of  $\epsilon$  as

$$H^*(\eta, \xi) = H_0^*(\eta, \xi) + \epsilon H_1^*(\eta, \xi) + \dots \quad (11)$$

and parameter  $\tau$  is introduced by the auxiliary equation

$$\frac{d\eta_j}{d\tau} = -\frac{\partial H_0^*}{\partial \xi_j}, \quad (12)$$

$$\frac{d\xi_j}{d\tau} = \frac{\partial H_0^*}{\partial \eta_j}, \quad (13)$$

where  $j = 1, 2, 3$  and hence  $H_0^* = \text{const}$ . The  $H_k^*$ s in the power series (11) are obtained (details are given in [1,2]) by

$$\begin{aligned}
 H_0^* &= \frac{1}{2}(\eta_1^2 + \eta_2^2 + \omega_1^2 \xi_1^2 + \omega_2^2 \xi_2^2 + \omega_3^2 \xi_3^2) \\
 H_1^* &= [H_1(\eta, \xi)]_s \\
 S_1 &= \int [H_1(\eta, \xi)] - H_1^* d\tau \\
 H_2^* &= \frac{1}{2} \{H_1 + H_1^*, S_1\}_s \\
 S_2 &= \int \left[ \frac{1}{2} \{H_1 + H_1^*, S_1\} - H_2^* \right] d\tau \\
 H_3^* &= \frac{1}{2} \{H_1 + H_1^*, S_2\}_s + \frac{1}{2} \{H_2 + H_2^*, S_1\}_s \\
 &\quad + \frac{1}{12} \{ \{H_1 - H_1^*, S_1\}, S_1 \}_s, \tag{14}
 \end{aligned}$$

where the subscript  $s$  stands for the average value which is defined for a function  $A$  as

$$A_s = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t A(\tau) d\tau \tag{15}$$

and for a periodic function with period  $T$ , the above equation becomes

$$A_s = \frac{1}{T} \int_0^T A(\tau) d\tau. \tag{16}$$

### 3. Semiclassical eigenvalues

First we obtain  $H_0^*$ ,  $H^*$  as analytic expressions and equivalent constants of motion for two non-Hermitian systems given in eqs (1) and (2). The above Hamiltonians are found to be functions of new variables  $\xi_1, \xi_2, \xi_3, \eta_1, \eta_2$  and  $\eta_3$  only in the form  $\xi_1^2 + \eta_1^2/\omega_1^2$ ,  $\xi_2^2 + \eta_2^2/\omega_2^2$ , and  $\xi_3^2 + \eta_3^2/\omega_3^2$ . These transformed Hamiltonians are merely the Birkhoff normal forms [18,19] of the original Hamiltonians.

#### 3.1 Eigenvalues of $H_a$

The Hamiltonian  $H_a$  in (1) is PT symmetric and is known to have all eigenvalues real. Assuming  $\omega_i = \omega_j + \omega_k$  for all  $i \neq j \neq k$ , and  $\omega_1, \omega_2$  and  $\omega_3$  are not commensurable with each other,  $H_0^*(\eta, \xi)$  and  $H^*(\eta, \xi)$  are found for the above system as

$$H_a^* = \frac{1}{2} \left[ \sum_{i=1}^3 c_i \omega_i^2 \right] + \frac{g^2}{2} \beta_a, \tag{17}$$

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where

$$\beta_a = \frac{\{c_1 c_3(-\omega_1^2 + \omega_2^2 - \omega_3^2) + c_2 c_3(\omega_1^2 - \omega_2^2 - \omega_3^2) + c_1 c_2(-\omega_1^2 - \omega_2^2 + \omega_3^2)\}}{(\omega_1 - \omega_2 - \omega_3)(\omega_1 + \omega_2 - \omega_3)(\omega_1 - \omega_2 + \omega_3)(\omega_1 + \omega_2 + \omega_3)}$$

and

$$c_1 = (\xi_1^2 + \eta_1^2/\omega_1^2), \quad c_2 = (\xi_2^2 + \eta_2^2/\omega_2^2), \quad c_3 = (\xi_3^2 + \eta_3^2/\omega_3^2)$$

$$H_{a0}^* = \frac{1}{2} (\eta_1^2 + \eta_2^2 + \eta_3^2 + \omega_1^2 \xi_1^2 + \omega_2^2 \xi_2^2 + \omega_3^2 \xi_3^2). \quad (18)$$

When  $g = 0$ , this system is separable and all the trajectories are periodic. Therefore, classical actions can be defined as  $\oint_C p_x dx$ ,  $\oint_C p_y dy$  and  $\oint_C p_z dz$  using periodic orbits. When non-separable real Hermitian 3D systems are regular (non-chaotic) classical actions can be defined by integrating over topologically independent paths [20–22] which are closed curves. However, when  $g$  is complex, it is evident from numerical calculation of trajectories that the Hamiltonian  $H_a$  does not constitute such close curves and hence actions cannot be defined in the usual manner.

With the transformed coordinates and momenta,  $\xi_i, \eta_i$  ( $i = 1, 2, 3$ ) which are the solutions of eqs (12) and (13), we can evaluate classical action integrals  $I_i = \oint \eta_i d\xi_i$  exactly and they are found to be

$$I_i = (\xi_i^2 + \eta_i^2/\omega_i^2)\omega_i\pi, \quad (19)$$

where  $i = 1, 2, 3$ . Using eq (19), we can write the quantization conditions for the above system as

$$I_i = \left(n_i + \frac{1}{2}\right)\hbar, \quad (20)$$

where  $i = 1, 2, 3$  and  $n_i$ 's are quantum numbers. Hence we obtain the following analytic expression for semiclassical energy eigenvalues of  $H_a$ .

$$E_{n_1, n_2, n_3}^a = \sum_{i=1}^3 \left(n_i + \frac{1}{2}\right)\hbar\omega_i + \frac{g^2}{2}\beta_a \quad (21)$$

$$\begin{aligned} \beta_a = & \left( \left(n_1 + \frac{1}{2}\right) \left(n_3 + \frac{1}{2}\right) (-\omega_1^2 + \omega_2^2 - \omega_3^2) \omega_2 \right. \\ & + \left(n_2 + \frac{1}{2}\right) \left(n_3 + \frac{1}{2}\right) (\omega_1^2 - \omega_2^2 - \omega_3^2) \omega_1 \\ & \left. + \left(n_1 + \frac{1}{2}\right) \left(n_2 + \frac{1}{2}\right) (-\omega_1^2 - \omega_2^2 + \omega_3^2) \omega_3 \right) \\ & / \omega_1 \omega_2 \omega_3 (\omega_1 - \omega_2 - \omega_3) (\omega_1 + \omega_2 - \omega_3) \\ & \times (\omega_1 - \omega_2 + \omega_3) (\omega_1 + \omega_2 + \omega_3). \end{aligned}$$

Eigenvalues obtained from the above equations are compared with eigenvalues calculated by Rayleigh–Schroedinger perturbation theory and numerical energies. The results are presented in table 1.

**Table 1.** First ten eigenenergies of  $V(x) = \frac{1}{2}(\omega_1^2 x_1^2 + \omega_2^2 x_2^2 + \omega_3^2 x_3^2) + igx_1 x_2 x_3$  where  $\omega_1 = 0.7, \omega_2 = 1.3, \omega_3 = 1.2185$  and  $g = 0.05$  are calculated using Lie transform method. Numerical eigenenergies are obtained by diagonalizing the Hamiltonian in harmonic oscillator basis-set.

$n_1$	$n_2$	$n_3$	Numerical	Lie transform	RS perturbation
0	0	0	1.6093	1.6096	1.6093
1	0	0	2.3096	2.3098	2.3093
0	0	1	2.8283	2.8285	2.8278
0	1	0	2.9099	2.9101	2.9093
2	0	0	3.0098	3.0100	3.0093
1	0	1	3.5287	3.5289	3.5278
1	1	0	3.6105	3.6107	3.6103
3	0	0	3.7101	3.7103	3.7093
0	0	2	4.0472	4.0475	4.0463
0	1	1	4.1296	4.1298	4.1278

It is evident from table 1 that the semiclassical eigenenergies are in good agreement with numerical quantum eigenvalues and the second-order Lie transform method produced more accurate eigenenergies than the second-order RS perturbation theory.

### 3.2 Eigenvalues of $H_b$

When all the parameters,  $\omega_1, \omega_2, \omega_3, \lambda, \mu, \alpha$  and  $\beta$  in  $H_b$  are real, the system is PT symmetric whereas, if  $\lambda$  and  $\mu$  are not pure imaginary and  $\alpha$  and  $\beta$  are non-real, the system is not pseudo-Hermitian. In the former case, the system has real and positive eigenvalues while for the latter case the system will have complex eigenvalues. On the other hand, when the system is not pseudo-Hermitian, the classical trajectories are found to be neither periodic nor quasi-periodic. However, as in the case of  $H_a$ , we obtain expressions for  $H_b^*$  and  $H_{0b}^*$

$$H_b^* = \frac{1}{2} \left[ \sum_{i=1}^3 c_i \omega_i^2 \right] + \beta_b, \quad (22)$$

where

$$\begin{aligned} \beta_b = & -\frac{15}{4} \left\{ \frac{\lambda^2 \eta^2}{\omega_1^2} c_1^2 + \frac{\mu^2 \xi^2}{\omega_2^2} c_2^2 \right\} \\ & + c_1 c_2 \left\{ \frac{2\lambda^2}{(\omega_1^2 - 4\omega_2^2)} - \frac{3\lambda^2 \alpha}{\omega_1} \right\} + c_2 c_3 \left\{ \frac{2\mu^2}{(\omega_2^2 - 4\omega_3^2)} - \frac{3\mu^2 \beta}{\omega_2} \right\} \\ & + 2 \left\{ \omega_2^4 c_2^2 \frac{\lambda^2 (\omega_2^2 - 3\omega_1^2/8)}{\omega_1^2 \omega_2^4 (\omega_1^2 - 4\omega_2^2)} + \omega_3^2 c_3^2 \frac{\mu^2 (\omega_3^2 - 3\omega_2^2/8)}{\omega_2^2 \omega_3^4 (\omega_2^2 - 4\omega_3^2)} \right\} \\ H_{b0}^* = & \frac{1}{2} (\eta_1^2 + \eta_2^2 + \eta_3^2 + \omega_1^2 \xi_1^2 + \omega_2^2 \xi_2^2 + \omega_3^2 \xi_3^2). \end{aligned} \quad (23)$$

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Eigenenergies  $E_{n_1, n_2, n_3}^b$  of this system are given by

$$E_{n_1, n_2, n_3}^b = \frac{1}{2} \left[ \sum_{i=1}^3 (\xi_i^2 + \eta_i^2 / \omega_i^2) \omega_i^2 \right] + \beta_b,$$

where

$$\begin{aligned} \beta_b = & -\frac{15}{4} \left\{ \frac{\lambda^2 \eta^2}{\omega_1^4} \left( n_1 + \frac{1}{2} \right)^2 + \frac{\mu^2 \zeta^2}{\omega_2^4} \left( n_2 + \frac{1}{2} \right)^2 \right\} \\ & + \left( n_1 + \frac{1}{2} \right) \left( n_2 + \frac{1}{2} \right) \left\{ \frac{2\lambda^2}{\omega_1 \omega_2 (\omega_1^2 - 4\omega_2^2)} - \frac{3\lambda^2 \alpha}{\omega_1^2 \omega_2} \right\} \\ & + \left( n_2 + \frac{1}{2} \right) \left( n_3 + \frac{1}{2} \right) \left\{ \frac{2\mu^2}{\omega_2 \omega_3 (\omega_2^2 - 4\omega_3^2)} - \frac{3\mu^2 \beta}{\omega_2^2 \omega_3} \right\} \\ & + 2 \left\{ \omega_2^2 \left( n_2 + \frac{1}{2} \right)^2 \frac{\lambda^2 (\omega_2^2 - 3\omega_1^2/8)}{\omega_1^2 \omega_2^4 (\omega_1^2 - 4\omega_2^2)} \right. \\ & \left. + \omega_3^2 \left( n_3 + \frac{1}{2} \right)^2 \frac{\mu^2 (\omega_3^2 - 3\omega_2^2/8)}{\omega_2^2 \omega_3^4 (\omega_2^2 - 4\omega_3^2)} \right\}. \end{aligned}$$

It is evident from tables 2 and 3 that the semiclassical eigenenergies are in good agreement with numerical quantum eigenvalues regardless of the hermiticity of the Hamiltonians and whether the trajectories are periodic or not.

**Table 2.** First ten eigenenergies of  $V(x) = \frac{1}{2}(\omega_1^2 x_1^2 + \omega_2^2 x_2^2 + \omega_3^2 x_3^2) + i\lambda(x_1 x_2^2 + \alpha x_1^3) + i\mu(x_2 x_3^2 + \beta x_3^3)$  where  $\omega_1 = 0.7$ ,  $\omega_2 = 1.3$ ,  $\omega_3 = 1.0$ ,  $\lambda = -0.1$ ,  $\mu = -0.1$ ,  $\alpha = 0.1$  and  $\beta = 0.1$  are calculated using Lie transform method. Numerical eigenenergies are obtained by diagonalizing the Hamiltonian in harmonic oscillator basis-set.

$n_1$	$n_2$	$n_3$	Numerical	Lie transform	RS perturbation
0	0	0	1.506	1.5069	1.5061
1	0	0	2.2139	2.2151	2.2139
0	0	1	2.5134	2.5146	2.5139
0	1	0	2.8262	2.8279	2.8271
2	0	0	2.9247	2.9265	2.9247
1	0	1	3.2211	3.2229	3.2217
0	0	2	3.5238	3.5261	3.5219
1	1	0	3.5441	3.5463	3.5451
3	0	0	3.6383	3.641	3.5726
0	1	1	3.8412	3.8437	3.8429

**Table 3.** First ten eigenenergies of  $V(x) = \frac{1}{2}(\omega_1^2 x_1^2 + \omega_2^2 x_2^2 + \omega_3^2 x_3^2) + i\lambda(x_1 x_2^2 + \alpha x_1^3) + i\mu(x_2 x_3^2 + \beta x_2^3)$  where  $\omega_1 = 0.7$ ,  $\omega_2 = 1.3$ ,  $\omega_3 = 1.0$ ,  $\lambda = -0.1$ ,  $\mu = -0.1$ ,  $\alpha = 0.1i$ , and  $\beta = 0.1i$  are calculated using Lie transform method. Numerical eigenenergies are obtained by diagonalizing the Hamiltonian in harmonic oscillator basis-set.

$n_1$	$n_2$	$n_3$	Numerical	Lie transform	RS perturbation
0	0	0	1.503 + 0.002i	1.504 + 0.002i	1.503 + 0.002i
1	0	0	2.201 + 0.005i	2.203 + 0.005i	2.202 + 0.005i
0	0	1	2.510 + 0.003i	2.511 + 0.003i	2.510 + 0.003i
0	1	0	2.819 + 0.006i	2.820 + 0.006i	2.819 + 0.006i
2	0	0	2.897 + 0.009i	2.898 + 0.009i	2.898 + 0.009i
1	0	1	3.209 + 0.006i	3.210 + 0.006i	3.209 + 0.006i
0	0	2	3.520 + 0.004i	3.522 + 0.003i	3.517 + 0.003i
1	1	0	3.521 + 0.015i	3.523 + 0.016i	3.522 + 0.016i
3	0	0	3.589 + 0.012i	3.591 + 0.012i	3.612 - 0.015i
0	1	1	3.832 + 0.008i	3.834 + 0.008i	3.833 + 0.008i

#### 4. Concluding remarks

In this paper, we studied two 3D non-Hermitian complex Hamiltonians,  $H_a$  and  $H_b$  with classical Lie transform method. The first Hamiltonian  $H_a$  is PT symmetric when  $g$  is real and all the low energy levels are found to be real and positive [16]. In this study it was found that classical phase space of  $H_a$  contains quasi-periodic trajectories. The semiclassical energies were obtained as algebraic expressions and semiclassical eigenenergies are found to be in very good agreement with numerical quantum eigenenergies. The second-order Lie transform method produced more accurate eigenenergies than the second-order RS perturbation theory. The second Hamiltonian  $H_b$  is PT symmetric when  $\lambda, \mu, \alpha$  and  $\beta$  are real and low level quantum eigenenergies are found to be real and positive. As for  $H_a$ , semiclassical energies of this system are obtained as an approximate algebraic expression and semiclassical eigenenergies are found to be in very good agreement with numerical quantum eigenenergies. When  $\lambda, \mu$  are real and  $\alpha$  and  $\beta$  are complex, Hamiltonian is not pseudo-Hermitian and the entire quantum eigenenergy spectrum is complex. In this case, the classical trajectories are found to be non-quasi-periodic for all the energies. However, the semiclassical eigenenergies are found to be in very good agreement with numerical quantum eigenenergies.

In this study we found that the Lie transform based semiclassical method can be applied to obtain semiclassical eigenvalues of multidimensional non-Hermitian Hamiltonian systems accurately. The validity of the method is independent of the existence of the classical quasi-periodic motion at low energies.



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