

RESEARCH ARTICLE

Semiclassical quantization of non-Hermitian 2-D systems: Classical (Lie transform) Perturbation theory

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Revised: 20 August 2008 ; Accepted: 24 November 2008

Abstract: Both real and complex semiclassical eigen energies of two dimensional non-Hermitian Hamiltonian systems are obtained by classical (Lie transform) perturbation theory requiring the action variables I_1 and I_2 to satisfy the quantization condition $I_1=(n_1+(1/2))\hbar$ and $I_2=(n_2+(1/2))\hbar$ respectively where n_1, n_2 are integers. Classical perturbation theory with Lie transform makes classical trajectories, which are non-periodic or non-quasi-periodic, periodic. It was observed that this method produces accurate eigen energies even when classical trajectories are not periodic or quasi-periodic. Eigen energies obtained by classical perturbation theory are compared with the same, determined by Rayleigh-Schroedinger perturbation theory

Keywords: Lie transform, non-Hermitian systems, semiclassical quantization

INTRODUCTION

Real non-separable multidimensional Harmonic Oscillator Systems have been widely used in the past for investigating classical chaos and its manifestation in quantum mechanics in Hamiltonian systems¹⁻¹². Further more, semiclassical investigations of these oscillators provide insight into the various experiments related to the intramolecular energy transfer and understanding of the nature and meaning of intramolecular randomization¹³. Although non-Hermitian multidimensional Harmonic oscillator systems do not provide such a practical insight yet, semiclassical investigations of non-Hermitian complex Hamiltonian systems are important from both the fundamental and practical point of view. In the first place they may expose important clues hidden in the correspondence between classical and quantum mechanics, especially when classical motion becomes chaotic or PT symmetry of quantum states are spontaneously broken. Secondly, they provide powerful

tools for calculations of highly excited energy spectra of the multidimensional complex systems. Particularly, when action variables or eigen energy expressions are available in analytic form, it is possible to have a better understanding on the classical behaviour, the semiclassical quantization and the semiclassical limit.

Classical perturbation theory based on Lie transforms has been used to obtain constants of motion of 2-D coupled Harmonic oscillator systems^{14,15} and to determine semiclassical eigen energies and linking quantum avoided crossing with classical chaos in real Hermitian systems in the past^{16,17}. Classical motion of 1-D non-Hermitian Hamiltonian systems has been studied in several investigations¹⁻²¹. In this paper, we use Lie transforms to investigate the classical frequencies and real and complex semiclassical eigen values of 2-D non Hermitian Hamiltonian systems analytically. In particular, we study two Hamiltonians, H_a and H_b , which are non Hermitian and classical trajectories of H_b which do not have periodic or quasi periodic trajectories,

$$H_a = (1/2) [p_1^2 + p_2^2 + \omega_1^2 x_1^2 + \omega_2^2 x_2^2] + igx_1 x_2^2 \quad \dots (1)$$

and

$$H_b = (1/2) [p_1^2 + p_2^2 + \omega_1^2 x_1^2 + \omega_2^2 x_2^2] + igx_1^2 x_2^2 \quad \dots (2)$$

H_a is PT symmetric while H_b is neither PT symmetric nor pseudo-Hermitian. Using Lie transform, we find integrable Hamiltonians which are the integrable approximates to non-integrable Hamiltonians H_a and H_b . Outline of the paper is as follows. In section I, we describe the classical perturbation theory (Lie transform) method and apply it for the above systems to obtain approximate integrable Hamiltonians. In section II, classical frequencies are

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obtained by solving the equation of motion in transformed coordinates. In section III, the semiclassical eigen values are calculated using classical perturbation theory and compares them with exact and Rayleigh-Schrodinger perturbation energies. Concluding remarks are given in section IV.

I Classical Lie canonical transform

In this section, first we describe the classical perturbation theory based on Lie canonical transformations. (For further details, see reference 14 & 15). Consider the Hamiltonian of the form

$$H = H_0 + \varepsilon H_1 \quad \dots (3)$$

where $H_0 = (1/2) [p_1^2 + p_2^2 + \omega_1^2 x_1^2 + \omega_2^2 x_2^2]$ and $H_1(x_1, x_2)$ makes the above Hamiltonian H non-separable and non-Hermitian. Hamilton's equation of motion for the above Hamiltonian is

$$\frac{dp_j}{dt} = -\frac{\partial H}{\partial x_j} \quad \dots (4)$$

and

$$\frac{dx_j}{dt} = \frac{\partial H}{\partial p_j} \quad \dots (5)$$

($j=1,2$).

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

$$p_j = \eta_j - \varepsilon \frac{\partial S_1}{\partial \xi_j} - \varepsilon^2 \frac{\partial S_2}{\partial \xi_j} - \frac{1}{2} \varepsilon^2 \left\{ \frac{\partial S_1}{\partial \xi_j}, S_1 \right\} + O(\varepsilon^3) \quad \dots (6)$$

and

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

where $\{ \}$ represents the Poisson bracket and equations of motion become

$$\frac{d\eta_j}{dt} = -\frac{\partial H^*}{\partial \xi_j} \quad \dots (8)$$

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

($j=1,2$) 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 τ which is introduced in (11) and (12). Now we expand H^* in a power series of ε as

$$H^*(\eta, \xi) = H_0^*(\eta, \xi) + \varepsilon H_1^*(\eta, \xi) + \dots (10)$$

and parameter τ is introduced by the auxiliary equation

$$\frac{d\eta_j}{d\tau} = -\frac{\partial H_0^*}{\partial \xi_j} \quad \dots (11)$$

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

($j=1,2$) and hence $H_0^* = \text{const}$. The H_k^* 's in the power series (10) are obtained (details are given in reference 14,15) by

$$H_0^* = \left(\frac{1}{2}\right) [\eta_1^2 + \eta_2^2 + \omega_1^2 \xi_1^2 + \omega_2^2 \xi_2^2]$$

$$H_1^* = [H_1(\eta, \xi)]_s$$

$$S_1 = \int [H_1(\eta, \xi) - H_1^*] d\tau \quad \dots (13)$$

$$H_2^* = \frac{1}{2} \{H_1 + H_1^*, S_1\}_s$$

$$S_2 = \int \left[\frac{1}{2} \{H_1 + H_1^*, S_1\} - H_2^* \right] d\tau$$

$$H_3^* = \frac{1}{2} \{H_1 + H_1^*, S_2\}_s + \frac{1}{2} \{H_2 + H_2^*, S_1\}_s + \frac{1}{12} \{ \{H_1 - H_1^*, S_1\}, S_1 \}_s$$

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

$$A_s = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t A(\tau) d\tau \quad \dots (14)$$

and for a periodic function with period T above equation becomes

$$A_s = \frac{1}{T} \int_0^T A(\tau) d\tau \quad \dots (15)$$

Now we obtain H_0^* , H^* and equivalent constants of motion for two non-Hermitian systems given in equations (1) and (2). The Hamiltonian H_a in (1) is PT symmetric and known to have all eigen values real. Assuming ω_1 is not commensurable with ω_2 , $H_0^*(\eta, \xi)$ and $H^*(\eta, \xi)$ are found for the above system as

$$H_a = \frac{1}{2} [(\xi_1^2 + \eta_1^2 / \omega_1^2) \omega_1^2 + (\xi_2^2 + \eta_2^2 / \omega_2^2) \omega_2^2] - \frac{g^2}{2\omega_1^2(\omega_1^2 - 4\omega_2^2)} \beta_a \dots (16)$$

where $\beta_a = \{ (\omega_2^2 - 3\omega_1^2/8)(\xi_2^2 + \eta_2^2/\omega_2^2)^2 + \omega_1^2(\xi_1^2 + \eta_1^2/\omega_1^2)(\xi_2^2 + \eta_2^2/\omega_2^2) \}$

$$H_{a0}^* = \frac{1}{2} (\eta_1^2 + \eta_2^2 + \omega_1^2 \xi_1^2 + \omega_2^2 \xi_2^2) \quad \dots (17)$$

This new system admits two first integrals, $H_{a0}^* = \text{const}$ and $H_a^* = \text{const}$ and they are equivalent to

$$(\xi_1^2 + \eta_1^2 / \omega_1^2) = \text{const} \quad \dots (18)$$

$$(\xi_2^2 + \eta_2^2 / \omega_2^2) = \text{const} \quad \dots (19)$$

Above equations (16), (18) and (19) will be used to quantize this system in the section III. Now we find similar expressions of H_0^* and H^* for the Hamiltonian systems H_b .

$$H_b = \frac{1}{2} \left[(\xi_1^2 + \eta_1^2 / \omega_1^2) \omega_1^2 + (\xi_2^2 + \eta_2^2 / \omega_2^2) \omega_2^2 \right] + \left. \frac{1}{4} \frac{(\xi_1^2 + \eta_1^2 / \omega_1^2)(\xi_2^2 + \eta_2^2 / \omega_2^2)}{\omega_1^2 \omega_2^3 (\omega_2^2 - \omega_1^2)} \left\{ ig + \frac{g^2}{2} \beta \right\} \right\} \dots (20)$$

where

$$\beta = \{ (3\omega_2^2 - 2\omega_1^2)(\xi_1^2 + \eta_1^2 / \omega_1^2) + (3\omega_1^2 - 2\omega_2^2)(\xi_2^2 + \eta_2^2 / \omega_2^2) \}$$

$$H_{b0} = \frac{1}{2} (\eta_1^2 + \eta_2^2 + \omega_1^2 \xi_1^2 + \omega_2^2 \xi_2^2) \quad \dots (21)$$

The above Hamiltonians are functions of new variables $\xi_1, \xi_2, \eta_1,$ and η_2 only in the form $\xi_1^2 + \eta_1^2 / \omega_1^2$ and $\xi_2^2 + \eta_2^2 / \omega_2^2$. These transformed Hamiltonians are merely the Borkhoff normal forms^{1,22} of the original Hamiltonians.

II Classical frequencies

In the previous section we expressed the Hamiltonians of two non-Hermitian systems given by (1) and (2) in terms of constants of motion using classical Lie transform method. Constants of motion for these two dimensional potentials, are

$$(\xi_1^2 + \eta_1^2 / \omega_1^2) = \text{const} - c_1 \quad \dots (22)$$

$$(\xi_2^2 + \eta_2^2 / \omega_2^2) = \text{const} - c_2 \quad \dots (23)$$

Therefore, functions of $\xi_1^2 + \eta_1^2 / \omega_1^2$ and $\xi_2^2 + \eta_2^2 / \omega_2^2$ are also constants of motion of those systems. In terms of c_1 and c_2 , Hamiltonians H_a and H_b become

$$H_a^* = \frac{1}{2} [c_1 \omega_1^2 + c_2 \omega_2^2] - \frac{g^2 \{ (\omega_2^2 - 3\omega_1^2 / 8) c_2^2 + \omega_1^2 c_1 c_2 \}}{2\omega_1^2 (\omega_1^2 - 4\omega_2^2)} \quad \dots (24)$$

$$H_b^* = \frac{1}{2} [c_1 \omega_1^2 + c_2 \omega_2^2] + \frac{1}{4} \frac{c_1 c_2 \{ ig + g^2 \{ (3\omega_2^2 - 2\omega_1^2) c_1 + (3\omega_1^2 - 2\omega_2^2) c_2 \} / 2 \}}{\omega_1^2 \omega_2^3 (\omega_2^2 - \omega_1^2)} \quad \dots (25)$$

respectively. Using equation (8) and (9), we write the equations of motion for the above systems in terms of c_1 and c_2 as

$$\frac{d^2 \xi_j}{dt^2} + \Omega_{k,j}^2 \xi_j = 0 \quad \dots (26)$$

where $k = \{a, b\}, j = \{1, 2\}$ and $\Omega_{k,j} = \frac{2}{\omega_j} \left(\frac{\partial H_k^*}{\partial c_j} \right)$. Frequencies $\Omega_{k,j}$ are independent of time as c_1 and c_2 are constants of motion. Therefore, the solutions of equation motion (26) are simply

$$\xi_j = \sqrt{c_j} \text{Cos}(\Omega_{k,j} t + \varphi) \quad \dots (27)$$

$$\eta_j = -\Omega_{k,j} \sqrt{c_j} \text{Sin}(\Omega_{k,j} t + \varphi)$$

where φ is an integration constant and

$$\Omega_{a,1} = \omega_1 - \frac{g^2 c_2}{\omega_1 (\omega_1^2 - 4\omega_2^2)}$$

$$\Omega_{a,2} = \omega_2 - \frac{2g^2 c_2 (\omega_2^2 - 3\omega_1^2 / 8)}{\omega_2 \omega_1^2 (\omega_1^2 - 4\omega_2^2)} - \frac{g^2 c_1}{\omega_2 (\omega_1^2 - 4\omega_2^2)} \quad \dots (28)$$

$$\Omega_{b,1} = \omega_1 + \frac{1}{2} \frac{c_2 \{ ig + \frac{g^2}{2} \{ (3\omega_2^2 - 2\omega_1^2) c_1 + (3\omega_1^2 - 2\omega_2^2) c_2 \} \}}{\omega_1^2 \omega_2^3 (\omega_2^2 - \omega_1^2)} + \frac{c_1 c_2 g^2 (3\omega_2^2 - 2\omega_1^2)}{4\omega_1^2 \omega_2^3 (\omega_2^2 - \omega_1^2)}$$

$$\Omega_{b,2} = \omega_2 + \frac{1}{4} \frac{c_1 \{ ig + \frac{g^2}{2} \{ (3\omega_2^2 - 2\omega_1^2) c_1 + (3\omega_1^2 - 2\omega_2^2) c_2 \} \}}{\omega_1^2 \omega_2^4 (\omega_2^2 - \omega_1^2)} + \frac{c_1 c_2 g^2 (3\omega_2^2 - 2\omega_1^2)}{4\omega_1^2 \omega_2^4 (\omega_2^2 - \omega_1^2)} \quad \dots (29)$$

It is important to note that Hamiltonians H_k^* ($k = \{a, b\}$) are integrable, while corresponding original Hamiltonians H_k are not. H_k^* are the integrable approximates to H_k . It is evident from the above expressions for the frequencies of oscillations $\Omega_{k,j}$, that the classical trajectories of the first Hamiltonian system is periodic with real frequencies. However, the frequencies of the second Hamiltonian H_b^* are complex and classical trajectories of that Hamiltonian are therefore non-periodic. Under the Lie transform, non-integrable Hamiltonians became integrable and quasi-periodic trajectories of the first pseudo Hermitian Hamiltonian became periodic. However, trajectories of the second non-pseudo Hermitian Hamiltonians did not become periodic. Then an important question to address is that whether the semiclassical quantization of the above complex non-Hermitian systems accurately produce the quantum eigen values as it does in the case of real Hermitian systems. This issue is addressed in the next section.

III Semiclassical eigen values

In order to find semiclassical energy eigen values of those three Hamiltonians, first we make the transformation to action variables as or $I_j = (\xi_j^2 + \eta_j^2 / \omega_j^2) \omega_j \pi$

$$I_1 = (\xi_1^2 + \eta_1^2 / \omega_1^2) \omega_1 \pi \quad \dots (30)$$

$$I_2 = (\xi_2^2 + \eta_2^2 / \omega_2^2) \omega_2 \pi \quad \dots (31)$$

Therefore, Hamiltonians in terms of action variable I_1 and I_2 are given by

$$H^{a,b}(I_1, I_2) = \frac{1}{2\pi} [I_1\omega_1 + I_2\omega_2] - \frac{2g^2}{\pi^2\omega_1^2\omega_2^2(\omega_1^2 - 4\omega_2^2)} \beta_{\dots} \quad (32)$$

$$H^b(I_1, I_2) = \frac{1}{2\pi} [I_1\omega_1 + I_2\omega_2] + \left. \frac{I_1 I_2}{\pi^3(\omega_2^2 - \omega_1^2)\omega_1^3\omega_2^4} \left\{ ig + \frac{g^2}{\omega_1\omega_2} \beta_b \right\} \right\} \dots \quad (33)$$

where $\beta_a = \{(\omega_2^2 - 3\omega_1^2/8)I_2^2 + I_1 I_2 \omega_1 \omega_2\}$ and $\beta_b = \{(3\omega_2^2 - 2\omega_1^2)I_1\omega_2 + (3\omega_1^2 - 2\omega_2^2)I_2\omega_1\}$

Now we quantize the systems H_a and H_b with the quantization conditions

$$I_1 = \left(n_1 + \frac{1}{2} \right) \hbar \quad \dots \quad (34)$$

$$I_2 = \left(n_2 + \frac{1}{2} \right) \hbar \quad \dots \quad (35)$$

where n_1 and n_2 are the two quantum numbers. In this way, we can quantize both non-Hermitian Hamiltonians discussed above. Now we derive expressions for quantum mechanical eigen energies by applying aforementioned quantization conditions.

Imposing conditions (34) and (35) on (32) and (33), we obtain the quantum eigen energy expressions for the Non-Hermitian systems defined in (1) and (2) respectively as

$$E^{a,n_1,n_2} = \left[\left(n_1 + \frac{1}{2} \right) \omega_1 + \left(n_2 + \frac{1}{2} \right) \omega_2 \right] - \left. \frac{2g^2}{\omega_1^2\omega_2^2(\omega_1^2 - 4\omega_2^2)} \beta_a \right\} \dots \quad (36)$$

$$E^{b,n_1,n_2} = \left[\left(n_1 + \frac{1}{2} \right) \omega_1 + \left(n_2 + \frac{1}{2} \right) \omega_2 \right] + \left. \frac{\left(n_1 + \frac{1}{2} \right) \left(n_2 + \frac{1}{2} \right)}{\omega_1^3\omega_2^4(\omega_2^2 - \omega_1^2)} \left\{ ig + \frac{g^2}{\omega_1\omega_2} \beta_b \right\} \right\} \dots \quad (37)$$

where now $\beta_a = \{(\omega_2^2 - 3\omega_1^2/8)(n_2 + 1/2)^2\omega_1^2 + (n_1 + 1/2)(n_2 + 1/2)\omega_1\omega_2\}$ and $\beta_b = \{(3\omega_2^2 - 2\omega_1^2)(n_1 + 1/2)\omega_2 + (3\omega_1^2 - 2\omega_2^2)(n_2 + 1/2)\omega_1\}$ and \hbar is taken as unity.

E^{a,n_1,n_2} and E^{b,n_1,n_2} in (36) and (37) are the quantum eigen energies of the systems (1) and (2) respectively and n_1 and n_2 are non negative integers (quantum numbers). Tables 1 and 2 contain the eigen energies calculated using second order Lie transform method and the second order Rayleigh-Schroedinger perturbation theory. For comparison purposes, exact eigen energies which are obtained by diagonalizing the Hamiltonian in Harmonic oscillator basis set are also included in each table.

Table 1: First ten eigen energies of $V(x) = (1/2)[\omega_1^2 x_1^2 + \omega_2^2 x_2^2 + igx_1x_2^2]$ where $\omega_1=0.7$, $\omega_2=1.3$ and $g=0.08$ are calculated using Lie transform method and the second order Rayleigh-Schroedinger (RS) perturbation theory. "Exact" eigen energies are obtained by diagonalizing the Hamiltonian in Harmonic oscillator basis set.

Exact	Lie transform	2 nd order RS Perturb
1.00137	1.00149	1.00138
1.70247	1.70261	1.7025
2.30981	2.31004	2.30992
2.40355	2.40373	2.40362
3.01305	3.0134	3.01329
3.10462	3.10485	3.10474
3.62548	3.62601	3.6259
3.71624	3.71677	3.71665
3.80567	3.80598	3.80586
4.33079	4.33162	4.33151

Table 2: First ten eigen energies $V(x) = (1/2)[\omega_1^2 x_1^2 + \omega_2^2 x_2^2 + igx_1x_2^2]$ of where $\omega_1=0.7$, $\omega_2=1.3$ and $g=0.05$ are calculated using Lie transform method and Rayleigh-Schroedinger (RS) perturbation theory. "Exact" eigen energies are obtained by diagonalizing the Hamiltonian in Harmonic oscillator basis set.

Exact	Lie Transform	2 nd order RS Perturb
1.0006 + 0.0137i	1.0005 + 0.0137i	1.0006 + 0.0137i
1.7026 + 0.0408i	1.7029 + 0.0412i	1.7027 + 0.0412i
2.3033 + 0.0406i	2.3027 + 0.0412i	2.3034 + 0.0412i
2.4064 + 0.0674i	2.4073 + 0.0687i	2.4067 + 0.0687i
3.0121 + 0.1210i	3.0125 + 0.1236i	3.0129 + 0.1236i
3.1117 + 0.0930i	3.1136 + 0.0962i	3.1128 + 0.0962i
3.6074 + 0.0669i	3.6066 + 0.0687i	3.6079 + 0.0687i
3.7258 + 0.1992i	3.7282 + 0.2060i	3.7283 + 0.2060i
3.8181 + 0.1174i	3.8219 + 0.1236i	3.8208 + 0.1236i
4.3255 + 0.1993i	4.3272 + 0.2060i	4.3283 + 0.2060i

The above two tables clearly show that the semiclassical eigen energies are in good agreement with exact quantum eigen values regardless of the Hermiticity of the Hamiltonians and whether the periods of the trajectories

are real or not. For the Hamiltonian H_b , the second order Rayleigh-Schrodinger (RS) perturbation theory produces same complex energies as the semiclassical energies calculated with Lie transform method.

IV Concluding remarks

In this paper, we studied two 2D non Hermitian complex Hamiltonians, H_a and H_b with Classical Lie transform method. The first Hamiltonian H_a is PT symmetric and the entire quantum energy spectrum is found to be real and positive. In this study it was found that classical phase space of H_a contains periodic trajectories and analytic expression for frequency of oscillations was obtained. Semiclassical energies are obtained as an algebraic expression and semiclassical eigen energies are found to be in very good agreement with exact quantum eigen energies.

The second Hamiltonian H_b is not even pseudo Hermitian. The entire quantum energy spectrum is complex. The classical frequencies are found to be complex and hence all the classical trajectories are non periodic. Since an action variable is intrinsically a concept associated with periodic motion, existence of action variable is directly linked with that of the periodic motion. However, semiclassical eigen energies based on quantization of the action variables in this system are found to be quite accurate although no trajectories of this system is periodic.

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