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Quantum and classical statistical mechanics of a class of non-Hermitian Hamiltonians

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Abstract

This paper investigates the thermodynamics of a large class of non-Hermitian, PT -symmetric oscillators, whose energy spectrum is entirely real. The spectrum is estimated by second-order WKB approximation, which turns out to be very accurate even for small quantum numbers, and used to generate the quantum partition function. Graphs showing the thermal behavior of the entropy and the specific heat, at all regimes of temperature, are given. To obtain the corresponding classical partition function, it turns out to be necessary in general to integrate over a complex 'phase space'. For the wrong-sign quartic, whose equivalent Hermitian Hamiltonian is known exactly, how this formulation arises, starting from the Hermitian case, is demonstrated explicitly.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The recent surge of interest in Hamiltonians which, although non-Hermitian, have a completely real spectrum, began with the pioneering paper by Bender and Boettcher [1], which gave strong numerical and analytical evidence that the spectrum of the class of Hamiltonians

$$H = p^2 - (ix)^N \quad (1)$$

was completely real and positive for $N \geq 2$ and attributed this reality to the (unbroken) PT symmetry of the Hamiltonian. Since then a large number of PT -symmetric models have been explored (see, e.g. [2]), and it was found that the phenomenon is rather general.

The natural metric arising in such theories is not positive definite, which precludes a straightforward physical interpretation in terms of probability amplitudes. However, it turns out that it is possible to construct [3] a grading operator C , which gives a positive-definite

metric $\eta_+ = PC$. In contrast to standard quantum mechanics, where the metric is the same for any Hermitian theory, here the metric is determined in each case by the Hamiltonian itself. In the Schrödinger wavefunction formulation of quantum mechanics, this metric appears explicitly in the calculation of Green's functions; however, in the path-integral of functional formulation, its role is much more subtle [4].

The class of Hamiltonians (1) can be thought of as a continuation in the exponent of the potential, starting with the harmonic oscillator, $N = 2$. A more general class of Hamiltonians [5, 6] is obtained by continuation off the x^{2M} oscillator:

$$H = p^2 + x^{2M}(ix)^\epsilon, \quad (2)$$

where $M = 1, 2, 3, \dots$; $\epsilon \geq 0$. They include the harmonic oscillator $H = p^2 + x^2$ ($M = 1, \epsilon = 0$) and non-Hermitian Hamiltonians such as $H = p^2 + ix^3$ ($M = 1, \epsilon = 1$), $H = p^2 - x^4$ ($M = 1, \epsilon = 2$) and $H = p^2 - x^6$ ($M = 2, \epsilon = 2$). The eigenvalue equation corresponding to (2) is

$$-\psi_n''(x) + x^{2M}(ix)^\epsilon \psi_n(x) = E_n \psi(x), \quad (3)$$

(throughout the text, $\hbar = k_B = 1$) where $\psi_n(x)$ is required to vanish as $|x| \rightarrow \infty$. As explained in [5, 6], when the total exponent $N \equiv 2M + \epsilon$ is greater than 4, the boundary condition can no longer be satisfied with x real, and one is obliged to analytically continue the eigenvalue equation (3) into the complex plane. Specifically it should be continued into the lower half x plane within a Stokes wedge symmetrically placed with respect to the imaginary axis³. When this is done, the energy spectrum turns out to be real, discrete and positive [1, 5, 6]. A rigorous proof of this property was eventually constructed by Dorey *et al* [7]. For reviews of the whole field of non-Hermitian Hamiltonians see [8].

In principle it is possible [9] to relate H by a similarity transformation to an equivalent Hermitian Hamiltonian h with the same energy spectrum. However, such a program is difficult to implement, and an exact form for h is available only in very few cases. It should be stressed that, unlike (3), the eigenvalue equation corresponding to h can always be solved on the real axis. Possible physical applications of these unusual Hamiltonians are beginning to emerge. We mention here the 'quantum brachistochrone', in which the standard lower bound for the transition time between two states can be circumvented [10] by a judicious interplay of Hermitian and non-Hermitian systems. How this could be achieved in practice has been recently discussed in [11]. In analog optical situations, where the refractive index plays the role of the potential, PT-symmetric systems have been shown to have unusual and interesting properties [12, 13]. Perhaps surprisingly, little attention has been paid so far to the thermodynamics of such systems. In the present paper we investigate the thermodynamics of the Hamiltonians of (2), which we hope will act as a template for the investigation of other non-Hermitian systems. As far as the quantum partition thermodynamics is concerned, we need only calculate the energy levels, on which the partition function depends. The high-temperature limit then probes the classical mechanics of these systems, and we use this to investigate how the classical partition function should be defined, which is not obvious *a priori*.

The paper is organized as follows. In section 2 we show that the energies E_n of (3) can be estimated to a high degree of accuracy, even for small values of n , using the WKB

³ This is why the superficially Hermitian Hamiltonians $H = p^2 - x^4$ and $H = p^2 - x^6$ are in fact non-Hermitian and *PT*-symmetric.

approximation including the subleading contribution. In section 3 we use the determined energy levels to evaluate numerically the canonical partition function, which then yields plots illustrating the thermal behavior of the entropy and the specific heat, at low, intermediate and high temperatures. The plots also show how the parameters M and ϵ affect these quantities. In the high-temperature limit, still using the WKB formula for E_n , we obtain a closed formula for the semiclassical partition function by integration over n .

This is then used, in section 4, as a tool for investigating how the semiclassical partition function Z_{cl} associated with H in (2) should be expressed as a ‘phase-space’ integral. In general this must differ from the usual real phase-space integral, which does not converge. The special case $H = p^2 - x^4$ (the wrong-sign quartic oscillator) is ideal for testing these ideas, because in this case one has an explicit form for the equivalent isospectral Hermitian Hamiltonian h . Thus one can start by calculating the semiclassical partition function using the real phase space associated with h , and then transform the variables to find the correct integral expression for Z_{cl} in terms of the variables appearing in H . Section 5 includes a summary and further discussion.

2. The WKB approximation for the spectrum

An extremely accurate approximation for the spectrum of H in (2) can be obtained using the WKB method including the subleading contribution. In [1, 5] the spectra were so calculated for $M = 1$. This section generalizes those results to the case $M > 1$.

One begins by solving the equation $x^{2M}(ix)^\epsilon = E$ to determine the turning points,

$$x_{\pm} = E^{1/N} e^{-i\pi(1/2 \mp M/N)}, \quad (4)$$

recalling that $N = 2M + \epsilon$. It should be pointed out that x_{\pm} are in the wedge mentioned in the previous section. For a given M , when $\epsilon = 0$, the turning points are $x_{\pm} = \pm E^{1/N}$. As ϵ increases from zero, these points migrate from the real axis toward the negative imaginary axis of the complex x plane.

The leading WKB contribution is obtained by imposing the condition

$$(n + 1/2)\pi = \int_{x_-}^{x_+} dx \sqrt{E - x^{2M}(ix)^\epsilon} \quad (5)$$

over a path for which the integration is real. Choosing the path as the ray going from x_- to 0, followed by that from 0 to x_+ , (5) can be recast as

$$(n + 1/2)\pi = 2 \sin(M\pi/N) E^{1/2+1/N} \int_0^1 ds \sqrt{1 - s^N}, \quad (6)$$

which yields the first factor in (8) below.

To calculate the subleading WKB contribution, instead of (5), one uses [5, 14]

$$(n + 1/2)\pi = (1/2i) \oint_C dx Q^{1/2} + (1/2i) \oint_C dx Q''/48Q^{3/2}, \quad (7)$$

where $Q(x) := x^{2M}(ix)^\epsilon - E$ and the contour C encircles counterclockwise the rays used to calculate the integration in (5). It follows then that

$$\begin{aligned} \frac{1}{2i} \oint_C dx \frac{Q''(x)}{48Q^{3/2}(x)} &= \frac{1}{24} N(N - 1) \sin(M\pi/N) \\ &\times E^{-1/2-1/N} \int_0^1 ds \frac{s^{N-2}}{(1 - s^N)^{3/2}}, \end{aligned}$$

Table 1. Energy levels E_n of the potential $|x|^4$. The successive columns are n , first- and second-order WKB, the numerical results from [15] and the approximation from [16].

n	WKB1	WKB2	Exact	Turschner
0	0.867 145 32	0.989 821 29	1.060 362 09	1.032 458
1	3.751 919 92	3.810 896 37	3.799 673 03	3.785 676
10	50.240 1523	50.256 2691	50.256 2545	50.254 484
50	407.868 707	407.874 363	407.874 363	407.873 65
100	1020.986 417	1020.989 992	1020.989 992	1020.989 538

Table 2. Energy levels E_n of the potential $-x^4$. The successive columns are n , first- and second-order WKB, and the numerical results from [1].

n	WKB1	WKB2	Exact
0	1.376 51	1.473 88	1.4771
1	5.9558	6.002 61	6.0033
2	11.769	11.8023	11.8023
3	18.4321	18.4588	18.4590

which when added to (6) yields (for large n)

$$E_n = \left(\frac{\Gamma(3/2 + 1/N) \sqrt{\pi} (n + 1/2)}{\sin(M\pi/N) \Gamma(1 + 1/N)} \right)^{2N/(N+2)} \times \left(1 + \frac{N(N - 1) \sin^2(M\pi/N) \cot(\pi/N)}{3\pi(n + 1/2)^2 (N + 2)^2} \right), \tag{8}$$

after identities involving products of gamma functions are used.

The energy spectrum corresponding to the Hamiltonian $p^2 + |x|^N$, which we consider for purposes of comparison, is obtained [5] by omitting the factors $\sin(M\pi/N)$ and $\sin^2(M\pi/N)$ in (8) (corresponding to $M = N/2$) and the results in [1, 5] are reproduced by setting $M = 1$ in (8). Tables 1 and 2 show that (8) is an excellent approximation for both the Hermitian and non-Hermitian versions even for small quantum numbers.

3. Quantum statistical mechanics

In quantum statistical mechanics the partition function is given by

$$Z(T) = \sum_{n=0}^{\infty} e^{-E_n/T}. \tag{9}$$

Note that this is exactly the same as it would be for a Hermitian Hamiltonian, with no appearance of the metric operator. As was first pointed out by Jakubský [17], this is due to the cyclic property of the trace in $Z = \text{Tr} e^{-H/T}$.

For the PT -symmetric oscillators we are considering, we use the second-order WKB approximation of (8) to evaluate the energies E_n . This is guaranteed to be accurate at high temperatures when the populations of states with high energies are appreciable, so that the relevant values of n are large. However, as we have illustrated above, the energies obtained are very accurate, even for small n , so the corresponding approximation for Z should also be accurate at low temperatures.

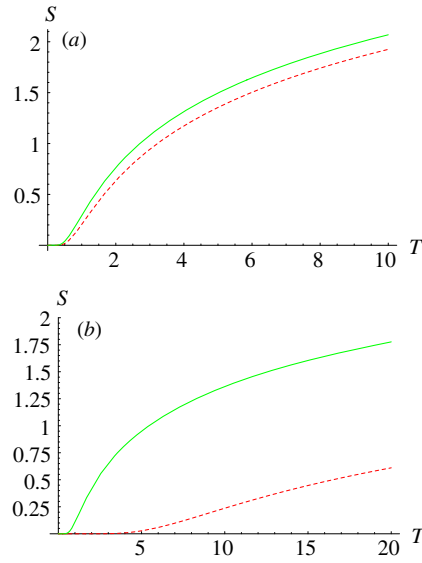


Figure 1. S versus T for $N = 3$ (a) and 10 (b), using the second-order WKB approximation (8) for the energies. In each case the solid curve (green) corresponds to $V = |x|^N$ and the dashed curve (red) to $V = x^2(ix)^{N-2}$ ($M = 1, \epsilon = N - 2$).

Once we have calculated $Z(T)$ we may evaluate other thermodynamic quantities in the standard way from the free energy $F = -T \log Z$, which yields the entropy $S = -dF/dT$, the internal energy $U = F + TS$ and the specific heat $C = dU/dT$. In figures 1 and 2 we illustrate the thermal behavior of S and C for $M = 1$ and various values of ϵ , and compare them with those obtained for the Hermitian potential $|x|^N$.

Apart from the case where $M = 1$ and $\epsilon = 0$ (the harmonic oscillator), there is no closed form for the summation in (9). However, a closed form can be obtained at high temperatures, where as mentioned above, (8) is most reliable. Working with the leading contribution in (8), since the subleading contribution is suppressed at large n , we obtain

$$Z(T) = \sum_{n=0}^{\infty} e^{-\beta E_0(2n+1)^{2N/(N+2)}}, \tag{10}$$

where E_0 denotes the first factor in (8) when $n = 0$, and $\beta := 1/T$. As $\beta E_0 \rightarrow 0$, the summation can be replaced by an integration,

$$Z_{cl}(T) = \int_0^{\infty} dn e^{-(\Theta/T)(n+1/2)^{2N/(N+2)}}, \tag{11}$$

where Θ is the characteristic temperature of the oscillator:

$$\Theta := \left[\frac{\Gamma(3/2 + 1/N)\sqrt{\pi}}{\sin(M\pi/N)\Gamma(1 + 1/N)} \right]^{2N/(N+2)}. \tag{12}$$

In fact, $\beta E_0 \rightarrow 0$ means $\Theta/T \ll 1$, i.e. one is dealing with the classical regime, as indicated by the change in notation from Z to Z_{cl} . A few manipulations in (11) lead to

$$Z_{cl}(T) = \Gamma(3/2 + 1/N) \left(\frac{T}{\Theta} \right)^{1/2+1/N}. \tag{13}$$

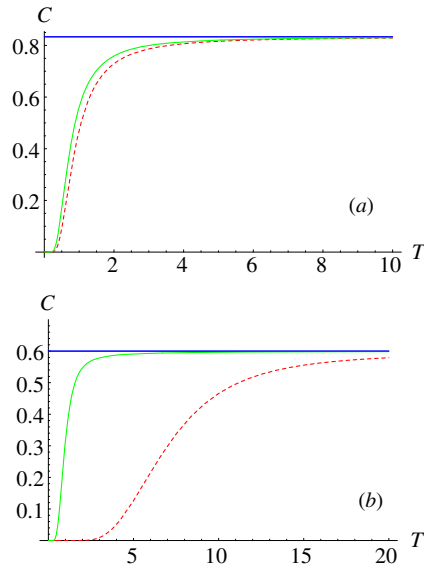


Figure 2. C versus T for $N = 3$ (a) and 10 (b), using the second-order WKB approximation (8) for the energies. In each case, the solid curve (green) corresponds to $V = |x|^N$ and the dashed curve (red) to $V = x^2(ix)^{N-2}$ ($M = 1, \epsilon = N - 2$).

By simple inspection, (13) yields the well-known expression T/Θ for the harmonic oscillator $N = 2$.

$Z_{cl}(T)$ in (13) leads to the entropy

$$S = [1/2 + 1/N][\log(T/\Theta) + 1] + \log \Gamma(3/2 + 1/N) \tag{14}$$

and specific heat

$$C = 1/2 + 1/N, \tag{15}$$

corresponding to the (classical) thermal behavior on the right-hand part of the plots. The characteristic temperature Θ in (12) gives the magnitude of the energy gap separating the first excited state and the ground state. As (12) clearly shows, for a given M , Θ is an unbounded increasing function of N . Since Θ separates the classical thermal behavior ((14) and (15)) from the quantum thermal behavior (corresponding in the plots to the drop toward zero as $T \rightarrow 0$), one sees that the larger the N the higher the temperature up to which the quantum behavior still prevails. These features are clear in the graphics.

It should be noted that

$$Z_{cl}(T) = Q_{cl}(N, T) \sin(M\pi/N), \tag{16}$$

where

$$Q_{cl}(N, T) = \frac{\Gamma(1 + 1/N)}{\sqrt{\pi} \beta^{1/2 + 1/N}} \tag{17}$$

is the semiclassical partition function corresponding to the Hamiltonian $p^2 + |x|^N$ [18]. As Z_{cl} and Q_{cl} are proportional to each other, they lead to the same thermodynamics as $T \rightarrow \infty$ (see plots), and in particular the specific heat is the same in both cases. Nevertheless, there is an important difference, namely, the characteristic temperature associated with Q_{cl} is bounded (it is given by Θ in (12) omitting $\sin(M\pi/N)$), and consequently their corresponding

thermodynamic functions may differ significantly at intermediate and small temperatures. For example, if $T \ll \Theta$, the corresponding specific heat would have the usual quantum behavior expressed by an exponential decay as $T \rightarrow 0$:

$$C \simeq \left(\frac{\Theta}{T}\right)^2 e^{-\Theta/T}, \quad (18)$$

whereas the same T might be much greater than the characteristic temperature associated with Q_{cl} , for which the classical behavior in (15) would be observed. (Strictly speaking, Θ in (18) should be replaced by the energy gap between the first excited state and the ground state, but this inaccuracy does not spoil the argument.)

4. Classical statistical mechanics

In standard classical statistical mechanics, with a Hermitian Hamiltonian, the partition function is given by integrating over the real phase space

$$\begin{aligned} Z_{\text{cl}}(T) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dp \int_{-\infty}^{+\infty} dx e^{-\beta H(p,x)} \\ &= \frac{1}{2\sqrt{\pi\beta}} \int_{-\infty}^{+\infty} dx e^{-\beta V(x)}, \end{aligned} \quad (19)$$

for $H = p^2 + V(x)$.

For the non-Hermitian Hamiltonians of (2) it is not immediately clear what is the correct formulation. For sufficiently small ϵ the integral of (19) is still convergent and indeed reproduces correctly the high-temperature limit of (16). However, for larger values of ϵ , for example $\epsilon > 1$ in the case $M = 1$, the integral along the real x -axis diverges, and in order to obtain a convergent result the contour of integration must be continued into the lower half of the complex x -plane.

The situation is similar, but not identical, to the Stokes wedges encountered in the quantum problem [1]. Thus, let us set $x = re^{-i\theta}$. The condition for convergence for large r is that $\text{Re } V > 0$, with $V = r^N e^{i(\pi\epsilon/2 - N\theta)}$, leading to

$$\cos \left[N \left(\frac{\pi}{2} - \theta \right) - M\pi \right] > 0.$$

This leads to wedges in the complex x -plane where the integral is convergent and other, forbidden, wedges where it is not. The forbidden wedges rotate downward and become more narrow as N increases, in a similar manner to Stokes wedges.

In the case $M = 1$, i.e. continuing away from the harmonic oscillator, the right-hand forbidden wedge is centered on $\theta_N = (\pi/2)(1 - 4/N)$ and has an opening angle π/N . There is a mirror image in the left-half plane. So for $N = 3$, the lower edge of the forbidden wedges lies precisely on the real axis, confirming that ix^3 is a limiting case. For $N = 4$, the forbidden wedges include the real axis, which is no longer viable as an integration contour. When $N = 5$ the upper edge of the wedges lies on the real axis, and thereafter the wedges lie entirely in the lower half plane. This latter situation is illustrated in figure 3 for $N = 6$. In this case the real axis is again a viable contour, but in fact it corresponds to the Hermitian potential $V = |x|^6$, whereas the hyperbolic contour is a possible contour for the non-Hermitian theory: it has been pushed off the real axis by the continuation in ϵ , and the two contours are separated by a forbidden region. There is in fact another forbidden wedge centered on the negative imaginary axis, which is avoided by the contour shown.

Moreover, these integrals are not only convergent, but they correctly reproduce the semiclassical result of (16). Thus, for example, in the case $N = 6$, if we integrate along

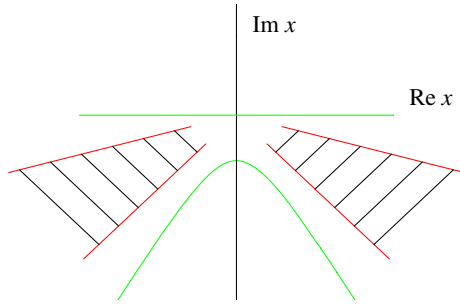


Figure 3. The classically forbidden wedges (hatched) for $N = 6$. The hyperbolic contour is a possible contour for the non-Hermitian $V = x^6$ ($M = 1, \epsilon = 4$), whereas integration along the real axis corresponds to $V = |x|^6$ ($M = 3, \epsilon = 0$).

the real axis we obtain $Q_{cl}(6, T)$, corresponding to the Hermitian case $M = 3, \epsilon = 0$, but if we integrate along the rays $x = \pm r \exp(\mp i\pi/3)$, the centers of the next allowed left and right wedges, we obtain precisely the extra factor $\cos(\pi/3) = \sin(\pi/N)$ required to give Z_{cl} for $M = 1$.

In principle, an alternative way of determining what is the correct expression for the classical partition function is to start with the definition in terms of the equivalent Hermitian Hamiltonian and make the appropriate changes of variables.

As mentioned in the introduction, in quantum mechanics a non-Hermitian Hamiltonian H with a completely real spectrum is related to an isospectral Hermitian Hamiltonian h by the similarity transformation [9]:

$$H = \rho^{-1} h \rho \equiv e^{\frac{1}{2}Q} h e^{-\frac{1}{2}Q}, \tag{20}$$

where the metric η_+ is written [3] in terms of the Hermitian operator Q as $\eta_+ = e^{-Q}$. The operator ρ is therefore Hermitian and positive definite. Thus we can certainly write Z_{cl} as

$$Z_{cl}(T) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dp e^{-\beta h(x,p)}. \tag{21}$$

From (20) we have the condition of quasi-Hermiticity on H :

$$H^\dagger = e^{-Q} H e^Q \equiv \eta H \eta^{-1}. \tag{22}$$

Similarly any observable A , with real expectation values, must also be quasi-Hermitian, i.e.

$$A^\dagger = e^{-Q} A e^Q \equiv \eta A \eta^{-1}. \tag{23}$$

This in turn means that A is related to a standard Hermitian counterpart a by the same similarity transformation:

$$A = e^{\frac{1}{2}Q} a e^{-\frac{1}{2}Q}.$$

We can use this latter equation to derive two different relations between H and h , namely

$$\begin{aligned} H(x, p) &= e^{\frac{1}{2}Q} h(x, p) e^{-\frac{1}{2}Q} = h(X, P), \\ H(X^\dagger, P^\dagger) &= e^{\frac{1}{2}Q} h(X^\dagger, P^\dagger) e^{-\frac{1}{2}Q} = h(x, p). \end{aligned} \tag{24}$$

It is the second of these identities that we need here, to write

$$Z_{cl}(T) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dp e^{-\beta H(X^\dagger, P^\dagger)}.$$

Now make the change of variables to $\xi \equiv X^\dagger$, $\pi \equiv P^\dagger$, to be treated here as classical variables. Thus, in the first instance (the Jacobian is 1),

$$Z_{\text{cl}}(T) = \frac{1}{2\pi} \iint_C d\xi d\pi e^{-\beta H(\xi, \pi)}, \tag{25}$$

where C is a contour in the complex (ξ, π) space determined parametrically by $\xi = X^\dagger(x, p)$, $\pi = P^\dagger(x, p)$. That is, the initial contour is ultimately determined by the metric η . Whether or not the contour can subsequently be deformed to a standard real phase space (ξ, π) is a matter to be determined for an individual Hamiltonian. From our preceding discussion it seems clear that this is not possible in general because of the presence of intervening forbidden wedges.

Note that the metric η does not appear explicitly as an integration measure in the integral representation (25) of the partition function, only through the form of the relationship between (ξ, π) and (x, p) . The issue of the role of η in path integrals has been addressed and clarified in [4, 19].

As mentioned above, there are very few cases where Q , and hence the relations between (x, p) and (ξ, π) , is known exactly. Apart from the rather trivial case of the Swanson model [20] (where in fact standard phase space can be used), a good example [21] within the class of Hamiltonians of (2) is the wrong-sign quartic $V = -x^4$.

A word of clarification is in order here. The original Hamiltonian in this case is really $H_z(z, p_z) = p_z^2 - z^4$, where the eigenvalue problem has to be posed on a complex contour in the appropriate Stokes wedges. It is only when a particular contour is chosen, with the parametrization $z = -2i\sqrt{(1 + ix)}$ in terms of the real variable x , that we obtain the non-Hermitian Hamiltonian $H(x, p)$ for which Q was found, namely

$$H(x, p) = \frac{1}{2}\{1 + ix, p^2\} - \frac{1}{2}p - \alpha(1 + ix)^2,$$

where, in the present case, $\alpha = 16$. The Q operator is

$$Q = -\frac{p^3}{3\alpha} + 2p,$$

which results, via the first equation of (24), in the equivalent Hermitian Hamiltonian

$$h(x, p) = \frac{p^4}{4\alpha} - \frac{1}{2}p + \alpha x^2.$$

This is still not a conventional Hamiltonian, but becomes so on taking the Fourier transform.

It is easily verified that using this $h(x, p)$ in (21) correctly gives the appropriate result ($M = 1$, $\epsilon = 2$) in (16). This is true whether or not one includes the linear term $-p/2$, which in fact is a quantum anomaly [22] proportional to \hbar .

If we now make the transformation to the variables $X^\dagger = \xi$ and $P^\dagger = \pi$, using the second equation of (24), we obtain

$$\begin{aligned} \pi &= p \\ \xi &= x + i \left(1 - \frac{p^2}{2\alpha}\right) \\ H(\xi, \pi) &= \frac{1}{2}\{1 + i\xi, \pi^2\} - \frac{1}{2}\pi - \alpha(1 + i\xi)^2. \end{aligned} \tag{26}$$

We now have an expression for Z_{cl} of the form of (25), in which the contour is given parametrically by (26) in terms of the real variables x and p . However, it is readily verified that there is no obstruction to deforming the contour to the real axis, so Z_{cl} can be expressed

as a real phase-space integral. But $H(\xi, \pi)$ has precisely the same form as $H(x, p)$, and we can take the reverse step to the original variables z and p_z . That is,

$$\begin{aligned} z &= -2i\sqrt{1+ix} \\ p_z &= p\sqrt{1+ix}, \end{aligned} \quad (27)$$

a canonical transformation from (x, p) to (z, p_z) . For any finite x , the argument of the variable p_z is less in modulus than $\pi/4$, so that it lies within the wedge including the real axis that guarantees convergence of the integral $\int dp_z \exp(-\beta p_z^2)$. Hence the p_z integral can be deformed to the real axis. However, for the z integration ($N = 4$), the contour cannot be so deformed because of an intervening forbidden wedge. This is in agreement with the results found previously when we performed the integrals over appropriately chosen rays, to obtain the correct semiclassical result of (16).

5. Discussion

To summarize, in this work we addressed the quantum and classical statistical mechanics of the class of non-Hermitian PT -symmetric oscillators of (2). These are in principle related by a similarity transformation to an equivalent Hermitian Hamiltonian h . However, for the quantum partition function $Z(T)$, one only needs the energy levels of H , which we evaluated using the WKB approximation including the first subleading correction. The main qualitative difference from the Hermitian oscillators ($M = N/2$) with potential $|x|^N$ turns out to be that because of the factor $\sin(M\pi/N)$ in the denominator the characteristic temperature $\Theta(M, N)$ of (12) grows without limit as N increases, so that the onset of semiclassical behavior is progressively delayed. At high temperatures, the entropy has the same form as that for the $|x|^N$ oscillator, except for the different value of Θ , and the specific heat is the same, depending only on N .

The semiclassical partition function $Z_{\text{cl}}(T)$ was determined in the first instance as the high-temperature limit of $Z(T)$. We then investigated how this result could be reproduced by a purely classical calculation and found that this could be achieved only by extending the classical phase-space integrations into the complex plane. Specifically, because of the simple dependence of H on p , the p integration can remain on the real axis, but the x -dependence means that the x integration can only be done within certain allowed wedges in the complex x plane, corresponding to different values of M . By integrating along the rays at the center of the allowed wedges, we verified that we indeed reproduced the semiclassical result of (16). In order to understand this from an alternative perspective, we considered the special case of the ‘upside-down’ quartic, the one example of the class (2) where h is known explicitly. Starting with the conventional Hermitian formulation for Z_{cl} in terms of h we implemented the similarity transformation to re-express it in terms of H , showing that indeed it required a complex contour in x of the type we had previously found.

It has been shown [23] that the classical Hamiltonian dynamics for systems of the type (1) and (2) can be formulated in a real 4-dimensional phase space, while a generalized canonical structure for non-Hermitian classical dynamics has recently been derived in [24]. It would be interesting to see how our results for the semiclassical partition function can be derived in those formalisms.

Acknowledgments

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