Feynman-Kleinert method applied to a complex PT-Potential

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1. Introduction:

According to some recent studies the energy spectrum of non-Hermitian Hamiltonians is real and positive[1-4]. This interest renewal to complex potentials is due to applications found in several research areas such as nuclear physics, quantum field theory, condensed matter physics, and biology.

The purpose of this letter is to study the simplest form of complex potentials that is, $V(x) = (1/4)x^2 + i\lambda x^3$, where λ is real and positive, via a systematic convergent variational perturbation theory for the path-integral representation of density matrices [4]. To our knowledge, it is for the first time that this formalism is used for such potentials according to the variational method. The variational perturbation theory [4,15] allows a very satisfactory approximation for path-integrals whenever the accurate analytical calculation of the propagator cannot be achieved. Taking into account the generalized smearing formula [4], which accounts for the effects of quantum fluctuations, we calculate the particle density in the complex potentials with a second order approximation.

This method can be schematized and summarized as follows. It is based upon a locally harmonic variational ansazt with the trial frequencies which are optimized differently for each expansion order. At high temperatures **T** , it is essential to give a special treatment to the fluctuations of the path average $\bar{x}_a = \int_0^\beta d\tau x(\tau)$ to deal with the free energy as the path performs violent fluctuations(k_B being the Boltzmann constant). The effects of these fluctuations may , however , easily be calculated at the end by a single numerical fluctuation integral . Variational perturbation expansions are performed for each positionx_a of the path average separately , yielding an Nth -order approximation $W_N(x_0)$ to the local free energy $V_{eff,cl}(x_0)$, called the effective classical potential [10]. In quantum mechanics, the partition function of a particle of mass ***M*** submitted to a one-dimensional potential V(x), can be expressed as a single integral over x_0 just as in classical statistics.

$$Z = \int_{-\infty}^{+\infty} \frac{dx_0}{\sqrt{2\pi\hbar^2\beta/M}} e^{-V_{eff,cl}(x_0)/k_B T} \qquad (1)$$

Having calculated , the Nth-order approximation to the partition function is obtained,

$$Z_N = \int_{-\infty}^{+\infty} \frac{dx_0}{\sqrt{2\pi\hbar^2\beta/M}} e^{-W_N(x_0)/k_B T} \qquad (2)$$

In the high temperature limit, $W_N(x_0)$ converges to the initial potential $V(x_0)$ for any order ***N***. the partition function in (1) can be written as

$$Z = \oint Dx \exp\left\{-A[x]/\hbar\right\} \qquad (3)$$

For the general particle action,

$$A[x] = \int_0^{\hbar\beta} d\tau \left[\frac{1}{2}M\dot{x}^2(\tau) + V(x(\tau))\right], \qquad (4)$$

Possesses the effective classical representation (1) with the effective classical potential

$$V_{eff,cl}(x_0) = -k_B T \ln\left[\left(\frac{2\pi\hbar^2}{MkBT}\right)^{1/2} \oint Dx\, \delta(x_0 - \bar{x}) \exp\left\{-A[x]/\hbar\right\}\right]. \qquad (5)$$

In the variational perturbation theory [4-10], the effective classical potential is expanded perturbatively around anx_0 -dependent harmonic system with the trial frequency $\Omega(x_0)$, and its optimization leads to the approximation$W_N(x_0)$ for $V_{eff,cl}(x_0)$.

2. Variational perturbation theory for density matrices:

To obtain a variational approximation for the density matrix, it is useful to split the general action (4) into a trial one for which the Euclidean propagator is known, and a remainder containing the original potential

$$A[x] = A^{\Omega,x_m}[x] + A_{int}[x], \qquad (6)$$

With an interaction term given by

$$A_{int}[x] = \int_0^{\hbar\beta} d\tau V_{int}(x(\tau)), \qquad (7)$$

Where x_m in (6) is determined by the minimum of the V(x) and $x_m = x_m(x_a, x_b)$, x_a and x_b are the end points, Ω is a trial frequency and $\beta = 1/k_B T$.

The interaction potential is the difference between the original V(x) and the one of a harmonic oscillator

$$V_{int}(x) = V(x) - \frac{1}{2}M\Omega^2[x - x_m]^2 \qquad (8)$$

The density matrix is defined by

$$\rho(x_b, x_a) = \frac{1}{Z}\tilde{\rho}(x_b, x_a) \qquad (9)$$

Where $\tilde{\rho}(x_b, x_a)$ is given by the following path-integral:

$$\tilde{\rho}(x_b, x_a) = \int_{(x_a,0)\to(x_b,\hbar/k_B T)} Dx \exp\left\{-A[x]/\hbar\right\} \qquad (10)$$

And the partition function is found from the trace of $\tilde{\rho}(x_b, x_a)$ as

$$Z = \int_{-\infty}^{+\infty} dx\, \tilde{\rho}(x, x) \qquad (11)$$

The path integration in (10) is evaluated by treating interaction (7) as a perturbation

$$\tilde{\rho}(x_b, x_a) = \tilde{\rho}_0^{\Omega,x_m}(x_b, x_a)\left[1 - \frac{1}{\hbar}\langle A_{int}[x]\rangle_{x_b,x_a}^{\Omega,x_m} + \frac{1}{2\hbar^2}\langle A_{int}^2[x]\rangle_{x_b,x_a}^{\Omega,x_m} - \ldots\ldots\right] \qquad (12)$$

Where $\tilde{\rho}_0^{\Omega,x_m}(x_b, x_a)$ is the path-integral for a harmonic oscillator [6]. The correlation functions in above equation can be decomposed into connected ones by going over to the cumulants. The series obtained is truncated to an N th-order approximatnt of the quantum-statistics density matrix [4]

$$\tilde{\rho}_N(x_b, x_a) = \tilde{\rho}_0^{\Omega,x_m}(x_b, x_a)\exp\left[\sum_{n=1}^{N}\frac{(-1)^n}{n!\hbar^n}\langle A_{int}^n[x]\rangle_{x_b,x_a}^{\Omega,x_m}\right] \qquad (13)$$

Which explicitly depends on both variational paramters Ω and x_m . An effective classical potential $V_{eff,cl}(x_a, x_b)$ is introduced, which governs the unnormalized density matrix

$$\tilde{\rho}(x_b, x_a) = \left(\frac{M}{2\pi\hbar^2\beta}\right)^{1/2}\exp\left[-\beta V_{eff,cl}(x_b, x_a)\right] \qquad (14)$$

Its N th-order approximation is obtained from the path-integral of a harmonic oscillator $\tilde{\rho}_0^{\Omega,x_m}(x_b, x_a)$, and from Eqs. (13), (14) via the cumulants expansion

$$W_N^{\Omega,x_m}(x_b, x_a) = \frac{1}{2\beta}\ln\frac{\sinh\hbar\beta\Omega}{\hbar\beta\Omega} + \frac{M\Omega}{2\hbar\beta\sinh\hbar\beta\Omega}\left\{(\tilde{x}_b^2 + \tilde{x}_a^2)\coth\hbar\beta\Omega - 2\tilde{x}_a\tilde{x}_b\right\} - \frac{1}{\beta}\sum_{n=1}^{N}\frac{(-1)^n}{n!\hbar^n}\langle A_{int}^n[x]\rangle_{x_a,x_b,c}^{\Omega,x_m} \qquad (15)$$

Which is optimized for each set of end points x_b and x_a in the variational parameters Ω^2 and x_m^N , the result being denoted by $W_N(x_b, x_a)$ .The following abbreviation $\tilde{x}(\tau) = x(\tau) - x_m$ is introduced. The optimal values $\Omega^2(x_b, x_a)$ and $x_m(x_b, x_a)$ are determined from the extreme conditions

$$\frac{\partial W_N^{\Omega,x_m}(x_b, x_a)}{\partial\Omega^2} = 0, \qquad \frac{\partial W_N^{\Omega,x_m}(x_b, x_a)}{\partial x_m} = 0. \qquad (16)$$

The solutions are denoted Ω^{2N} and x_m^N , both being functions of x_B and x_a . If no extrema are found, one has to look for the flattest region of function (15), where the lowest higher-order derivative disappears.

Kleinert and al.[4] found efficient formulas for evaluating expectation values of quantum-mechanical correlation functions of any power at atraction(7), in order to calculate the connected correlation functions in the variational perturbation expansion (15). The formulas can be written as

$$\langle A_{int}^n[x]\rangle_{x_a,x_b}^{\Omega,x_m} = \frac{1}{\rho_0^{\Omega,x_m}(x_a)}\prod_{l=1}^{n}\left[\int_0^{\hbar\beta} d\tau_l \int_{-\infty}^{+\infty} dz_l V_{int}(z_l + x_m)\right]\frac{1}{\sqrt{(2\pi)^{n+1}\det a^2}}\exp\left(-\frac{1}{2}\sum_{k,l=0}^{n} z_k a_{kl}^{-2} z_l\right),$$

with $z_0 = \tilde{x}_a$ and $\tau_0 = 0$. Here a^2 denotes a symmetric $(n+1)\times(n+1)$ matrix whose elements $a_{kl}^2 = a^2(\tau_k, \tau_l)$ are obtained from the harmonic Green function for periodic paths [2]:

The diagonal elements $a^2 = a^2(\tau, \tau')$ represent the fluctuation width$a_H^2 = (\hbar/2M\Omega)\coth(\hbar\Omega/2k_B T)$, which behaves in the classical limit as $a_{H,cl}^2 = k_B T/M\Omega^2$ and at zero temperature as $a_{H,0}^2 = \hbar/2M\Omega$.

It was shown on the basis of numerical studies that the energy of the Hamiltonian

$$H = p^2 + \frac{1}{4}x^2 + i\lambda x^3 \qquad (17)$$

Is real and positive[1]. It is claimed[1,2,16-19] that the reality and the positivity of the spectra are a consequence of PT-symmetry. Note that the parity operator acts as $P: p \to -p$ and $P: x \to -x$ and that antiunitarity timereversaloperation acts as$T: p \to -p, T: x \to x$ and $T: i \to -i$. The notion that PT-symmety can replace the much more restrictive condition of hermiticity has been worked out in the contex of quasi-exactly solvable quantum theories [20] and of new kinds of symmetry breaking in quantum field theory [21,22].

There are many applications of non-Hermitian PT-invariant Hamiltonians in physics. Hamiltonians rendered non-Hermitian by an imaginary external field have been used to study the delocalization transitions in condensed matter systems such as vortex flux-line depinning in type-II supercoductors [23] and to study population biology [24].

The large-order behavior of Rayleigh_Schrodinger perturbation theory for the ground-state energy of the complex PT-symmetric Hamiltonian (17) was studied [1].

Let us apply the systematic convergent variational perturbation theory [4] for the path-integral representation of density matrices to point particle moving in complex potentials [1,2].

In the second-order variational perturbation theory, the difference between the optimization procedures using one or two variational parameters becomes less signifiant. Thus we restrict ourselves to the optimization in $\Omega(x_a)$, and set $x_m = 0$ [4].

The second-order density is obtained as

$$\tilde{\rho}_2^{\Omega}(x_a) = \frac{1}{\sqrt{2\pi\hbar\beta}}\exp\left[-\beta W_2^{\Omega}(x_a)\right] \qquad (18)$$

with the second-order approximation of the effective classical potential,

$$W_2^{\Omega}(x_a) = \frac{1}{2}\ln\frac{\sinh\beta\Omega}{\beta\Omega} + \frac{\Omega}{\beta}x_a^2\tanh\frac{\beta\Omega}{2} + \frac{1}{\beta}\langle A_{int}[x]\rangle_{x_a,x_a}^{\Omega} - \frac{1}{2\beta}\langle A_{int}^2[x]\rangle_{x_a,x_a,c}^{\Omega}, \qquad (19)$$

Where

$$\langle A_{int}[x]\rangle_{x_a,x_a}^{\Omega} = \beta\left[g_0 + \frac{1}{2}C_\beta^{(1)}g_1 H_1\left(\frac{x_a}{\sqrt{2a_{00}^2}}\right) + \frac{1}{8}C_\beta^{(2)}g_2 H_2\left(\frac{x_a}{\sqrt{2a_{00}^2}}\right)\right]. \qquad (20)$$

$H_n(x)$ are the Hermite polynomials, and

$$g_0 = (1 - 2\Omega^2)\frac{a_{00}^2}{4}, \qquad g_1 = i\frac{3}{2}\lambda(2a_{00}^2)^{3/2}, \qquad g_2 = (1 - 2\Omega^2)a_{00}^2. \qquad (21)$$

the dimensionless functions$C_\beta^{(n)}$ are given by

$$C_\beta^{(n)} = \frac{1}{2^n\cosh^n\hbar\beta\Omega/2}\sum_{k=0}^{n}\binom{n}{k}\frac{\sinh\hbar\beta\Omega(n/2 - k)}{\hbar\beta\Omega(n/2 - k)}, \qquad (22)$$

And

$$\langle A_{int}^2(x)\rangle_{x_a,x_a,c}^{\Omega} = \langle A_{int}^2(x)\rangle_{x_a,x_a}^{\Omega} - \left(\langle A_{int}^2(x)\rangle_{x_a,x_a}^{\Omega}\right)^2.$$

The effective potential is obtained:

$$W_2^{\Omega}(x_a) = \frac{1}{2\beta}\frac{\sinh\beta\Omega}{\beta\Omega} + \frac{\Omega}{\beta}x_a^2\tanh\frac{\beta\Omega}{2} + \frac{(1 - 2\Omega^2)}{4}a_{00}^2 + \frac{C_\beta^2}{4}(x_a^2 - a_{00}^2)(1 - 2\Omega^2) + \frac{\lambda^2}{2\beta}F_1(x_a) - \frac{(1 - 2\Omega^2)^2}{32\beta}F_2(x_a) + i\frac{\lambda}{8\beta}(1 - 2\Omega^2)F_3(x_a). \qquad (23)$$

where

$$F_1(x_a) = -\frac{[3x_a^4 - 12a_{00}^2x_a^2 + 5a_{00}^4][\cosh^2\beta\Omega/2 + 2]^2 - 9\frac{a_{00}^2}{\Omega^4} - \frac{3[x_a^2 - a_{00}^2][\cosh^2\beta\Omega/2 + 2]}{2\Omega^6 a_{00}^4\sinh^2\beta\Omega/2}}{48\Omega^8 a_{00}^{10}\sinh^4\beta\Omega/2}$$
$$- \frac{[\cosh^3\beta\Omega/2 + 6\cosh\beta\Omega/2 - \cosh^3\beta\Omega/2 - 6\cosh 3\beta\Omega/2]}{12\Omega^5\sinh^3\beta\Omega/2}$$
$$+ \frac{3[x_a^2 - a_{00}^2][9\cosh^3\beta\Omega/2 - 10\cosh\beta\Omega/2 + \cosh 5\beta\Omega/2]}{16\Omega^5 a_{00}^2\sinh^3\beta\Omega/2}$$
$$+ \frac{[x_a^2 - a_{00}^2][58\cosh\beta\Omega + 4\cosh 2\beta\Omega - 69 + \cosh 4\beta\Omega + 6\cosh 3\beta\Omega]}{64\Omega^6 a_{00}^4\sinh^4\beta\Omega/2}$$
$$- \frac{[x_a^4 - 6a_{00}^2x_a^2 + 3a_{00}^4][101\cosh\beta\Omega/2 - 19\cosh 5\beta\Omega/2 - 81\cosh 3\beta\Omega/2]}{521 a_{00}^8\Omega^7\sinh^5\beta\Omega/2}$$
$$+ \frac{9a_{00}^4[\cosh 3\beta\Omega/2 - \cosh\beta\Omega/2]}{2\Omega^3\sinh\beta\Omega/2} - \frac{\cosh 7\beta\Omega/2}{521 a_{00}^8\Omega^7\sinh^5\beta\Omega/2},$$

$$F_2(x_a) = -\frac{[2x_a^2 - a_{00}^2][2\cosh\beta\Omega/2\sinh\beta\Omega/2 + \beta\Omega]^2}{32\Omega^6 a_{00}^6\sinh^4\beta\Omega/2} + \frac{2[\beta^2\Omega^2 + \sinh^2 3\beta\Omega/2 - \sinh^2\beta\Omega/2]}{8\Omega^4\sinh^2\beta\Omega/2}$$
$$+ \frac{[x_a^2 - a_{00}^2]}{32\Omega^5 a_{00}^4\sinh^3\beta\Omega/2}\left[-2\cosh\beta\Omega/2 + 4\beta\Omega\sinh\beta\Omega/2 + \cosh 3\beta\Omega/2 + \cosh 5\beta\Omega/2 + 4\beta\Omega\sinh 3\beta\Omega/2 + 4\beta^2\Omega^2 + \cosh\beta\Omega/2\right],$$

$$F_3(x_a) = \frac{[a_{00}^4x_a^3 + 3a_{00}^6x_a][\cosh^2\beta\Omega/2 + 2][2\cosh\beta\Omega/2\sinh\beta\Omega/2 + \beta\Omega]}{16\Omega^7\sinh^4\beta\Omega/2}$$
$$+ \frac{3a_{00}^{12}x_a[-1 + 2\beta\Omega\sinh\beta\Omega + \cosh 2\beta\Omega]}{8\Omega^8\sinh^2\beta\Omega/2}$$
$$+ \frac{2a_{00}^6x_a^3 - 5a_{00}^8x_a[-10 - \cosh\beta\Omega + 2\beta\Omega\sinh 2\beta\Omega]}{131\Omega^6\sinh^4\beta\Omega/2}$$
$$- \frac{5a_{00}^8x_a[20\beta\Omega\sinh\beta\Omega + \cosh 3\beta\Omega + 10\cosh 3\beta\Omega/2]}{131\Omega^6\sinh^4\beta\Omega/2}$$
$$+ \frac{3a_{00}^6x_a^3[-2\cosh\beta\Omega/2 + 4\beta\Omega(\sinh\beta\Omega/2 + \sinh 3\beta\Omega/2)]}{64\Omega^5\sinh^3\beta\Omega/2}$$
$$+ \frac{3a_{00}^6x_a[4(\beta\Omega)^2\cosh\beta\Omega/2 + \cosh 5\beta\Omega/2 + \cosh 3\beta\Omega/2]}{64\Omega^5\sinh^3\beta\Omega/2}$$

In the above derivation, we take into account the real parts in Eq. (23) to calculate $\tilde{\rho}_2^{\Omega}(x_a)$ via Eq. (11), the partition function Z_2 , and finally $E_K = \lim_{T\to 0}(-1/\beta\ln Z_2)$. Going further in the approximation by examining the second order in the imaginary part of Eq. (23), the imaginary parts that can be deduced are $\mathrm{Im}\left(W_2^{\Omega}(x_a)\right) \approx 0.00002$ for $\lambda = 0.015625$ and $\mathrm{Im}\left(W_2^{\Omega}(x_a)\right) \approx 0.00005$ for $\lambda = 2.0$.

On the other hand, for λ included between 0.015625 and 0.25 , $\mathrm{Im}\left(W_2^{\Omega}(x_a)\right)$ tends to zero. Based on their small values, the calculated imaginary parts can be neglected. In table 1, our results are compared with those obtained by the perturbation theory [1].

The results compiled in Table 1 show a great similarity between E_K and E_N obtained from perturbation theory [4]. The deviation with the λ value confirms this similarity: 0.07% for $\lambda = 0.5$ and 3% for $\lambda = 2.0$

λ	E_1	E_2	E_N	E_K
0.015625	0.50263	0.50263	0.50263	0.50263
0.03125	0.50998	0.50998	0.50998	0.50998
0.0625	0.53393	0.53393	0.53393	0.53393
0.125	0.59492	0.59492	0.59492	0.59492
0.25	0.71305	0.71384	0.71294	0.71295
0.5	0.91445	0.89035	0.90026	0.90092
1.0	1.0007	1.05817	1.16746	1.18978
2.0	3.16075	1.14032	1.53078	1.56208

Table 1:Energies for the potential in Eq.(19) for the different values of the parameter λ . The energies E_1, E_2, E_N and E_K are taken from [2]. The last column represent the values calculated by the variational perturbation theory for the density matrix

3. Conclusion:

In the conclusion, it can be said that the variational perturbation theory proposed by Kleinert and al.[4] affords reasonable and interesting results, when it is applied to the complexPT-symmetric Hamiltonian. Therefore, it can also be said that there is an effective agreement of numerical calculation studies accordingly with the mathematical point of view [3]. Finally, it is useful to have, for some PT-potential, the analytical solutions by the path-integral approach which is now being undertaken.

References

[1] C.M. Bender,G.V. Dunne, J. Math. Phys.40(1999)4616.
[2]M. Znojil, Phys. Lett. A 285 (2001) 7.
[3]K.C. Shin, math-ph/0201013.
[4] M. Bachmann, H. Kleinert, A. Pelster, Phys. Rev. 60(1999)3429.
[5] H. Kleinert, M. Meyer, Phys. Lett. A 184(1994)319.
[6] H. Kleinert, Path integrals in Quantum Mechanics, Statistics and Polymer Physics, 2nd ed.,World Scientific, Singapore, 1995
[7] H. Kleinert, W. Kürzinger, A. Pelster, J. Phys. A 31 (1987)8307.
[8] H. Kleinert, Phys. Lett. A 118 (1986) 267.
[9] W. Janke, H. Kleinert, Phys. Lett. A 118 (1986) 371.
[10] H. Kleinert, Phys. Lett. B 181 (1986) 324.
[11] M. Bentaiba, L.Chetouani, T.F. Hammann, Z. Naturforsch. 47A (1992) 1013.
[12] H. Kleinert, Phys. Lett. A 173 (1993) 332.
[13] M. Bentaiba, L.Chetouani, T.F. Hammann, Phys. Lett. A 189 (1994) 433.
[14] Kh. Nouicer, L. Chetouani, Acta Phys. Slovaca 49 (1999) 309.
[15] L.Chetouani, A.Chouchaoui,T.F. Hammann, Phys. Lett. A 204 (1995) 79
[16] C.M. Bender, G.V. Dunne, P.N. Meisinger, Phys.Lett. A 252 (1999) 272.
[17] C.M. Bender, S. Boettcher, Phys. Rev. Lett. 24 (1998) 5243.
[18] C.M. Bender, S. Boettcher, J. Phys. A: Math. Gen. 31 (1998) L273.
[19] C.M. Bender, G.V. Dunne, P.N. Meisinger, M.Simsek, Phys.Lett.A 281 (2001) 311;
[20] C.M. Bender, K.A. Milton, Phys. Rev. D 55 (1997) R 3255.
[21] C.M. Bender, K.A. Milton, Phys. Rev. D 57 (1998) 3595.
[22] C.R. Handy, math-ph/0104035.
[23] N. Hatano, D.R. Nelson, phys. Rev. Lett. 77 (1996) 570;
N. Hatano, D.R. Nelson, phys. Rev. B 56 (1997) 8651.
[24] D.R. Nelson, N.M. Shnerb, Phys. Rev. E 58 (1998) 1383.