

VARIATIONAL AND PERTURBATIVE METHOD FOR A THREE-BODY SYSTEM SUBMITTED TO A COMPLEX PT SYMMETRIC POTENTIAL

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(Received June 12, 2008; revised version received November 5, 2008)

The ground-state energy related to three particles subjected to a complex PT potential is calculated via the variational perturbation method for quantum statistical density matrices. It is found that the obtained energies are real and positive.

PACS numbers: 03.65.Ca, 31.15.Kb

1. Introduction

Various methods have been used to approximate the energy spectrum for complex potentials [1–10]. Zafar [11] has suggested a general ansatz for the energy-eigenstates when a complex one-dimensional PT symmetric potential possesses real spectrum. An high-order Rayleigh–Schrödinger perturbation theory was used [12] to obtain the perturbation series for ground-state energy of the one-dimensional complex cubic Hamiltonian $H = p^2 + x^2 + igx^3$. In an other work, low-lying energy levels corresponding to complex Hénon–Heiles potentials, have been calculated to very high order in perturbation theory [13].

In the Feynman integral formalism [14], there is a variational method called Feynman–Kleinert method [15], It has some formal similarities with the perturbative methods, applied in the Schrödinger formalism, but differs in the calculations. Kleinert [16,17] has introduced some improvements in the Feynman method in order to make it more performant. This technique is based on the matrix density expansion on the basis of the harmonic oscillator wave functions, and leads to very acceptable results in the case of anharmonic potentials [17].

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In this paper, we want to show that it is possible to use the Feynman–Kleinert method in order to determine, with a good accuracy, the ground state energy for three particles of equal mass subjected to a complex PT potential [24].

2. Mathematical method

Let us start with the standard partition function of a particle, with mass M , moving into potential $V(x)$ at a finite temperature T .

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

where the classical effective potential $V_{\text{eff,cl}}$ takes into account all quantum fluctuations [17] around the mean position $\bar{x}$ of the particle in the temperature interval $[0, \beta]$.

$$\bar{x} = \int_0^{\hbar\beta} x(\tau) d\tau,$$

where $\tau = it$ and $\beta = \frac{1}{k_b T}$, k_b being the Boltzmann constant.

On the other hand, the partition function Z can be written [17]:

$$Z = \int_{-\infty}^{+\infty} \frac{dx_0}{\sqrt{2\pi\hbar^2\beta/M}} \int Dx \delta(\bar{x} - x_0) \exp\left[-\frac{A[x]}{\hbar}\right]. \quad (2)$$

Where the measure of path integration for finite N is given by:

$$\int Dx = \prod_{j=1}^N \int_{-\infty}^{+\infty} \frac{dx_j}{\sqrt{2\pi\epsilon}}. \quad (3)$$

$A[x]$ is the Euclidian action of the particle.

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

By identifying (1) and (2) we have:

$$V_{\text{eff,cl}}(x_0) = -\frac{1}{\beta} \ln \left(\int Dx \delta(\bar{x} - x_0) \exp\left[-\frac{A[x]}{\hbar}\right] \right). \quad (5)$$

But it is impossible to calculate $V_{\text{eff,cl}}$ exactly for complicated forms of $V(x)$. Nonetheless, we can find an N -th order approximation $W_N(x_0)$ to the classical effective potential $V_{\text{eff,cl}}(x_0)$. The corresponding partition function Z_N is given by:

$$Z_N = \int_{-\infty}^{+\infty} \frac{dx_0}{\sqrt{2\pi\hbar^2\beta/M}} e^{-\beta W_N(x)}. \quad (6)$$

To obtain the best approximation W_N , the Euclidean action $A[x]$ of the system will be considered as the sum of two terms:

$$A[x] = A^{\Omega, x_m}[x] + A_{\text{int}}[x], \quad (7)$$

where $A^{\Omega, x_m}[x]$ is the trial action and, $A_{\text{int}}[x]$ is the interaction. They are given by:

$$A^{\Omega, x_m}[x] = \int_0^{\hbar\beta} \left[\frac{M}{2} \dot{x}^2 + \frac{M}{2} \Omega^2 (x - x_m)^2 \right] d\tau, \quad (8)$$

and

$$A_{\text{int}}[x] = \int_0^{\hbar\beta} \left[V(x) - \frac{M}{2} \Omega^2 (x - x_m)^2 \right] d\tau, \quad (9)$$

where x_m depends on the end points x_a and x_b .

Let us consider the matrix density defined as:

$$\rho(x_b, x_a) = \frac{1}{Z} \tilde{\rho}(x_b, x_a), \quad (10)$$

with

$$\tilde{\rho}(x_b, x_a) = \int_{(x_a, 0) \rightsquigarrow (x_b, \hbar\beta)} Dx \exp \left[-\frac{A[x]}{\hbar} \right] \quad (11)$$

replacing $A[x]$ by its expression (6), and expanding (10) in terms of $A_{\text{int}}[x]$, we obtain:

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

where $\tilde{\rho}_0^{\Omega, x_m}(x_b, x_a)$ is the density relating to the trial action $A^{\Omega, x_m}[x]$.

The different mean values appearing in (11) have been already calculated by Kleinert *et al.* [16], and they are given by:

$$\begin{aligned} \left\langle A_{\text{int}}^n [x] \right\rangle_{x_b, x_a}^{\Omega, x_m} &= \frac{1}{\rho_0^{\Omega, x_m}(x_a)} \prod_{l=1}^n \left[\int_0^{\hbar\beta} d\tau_l \int_{-\infty}^{+\infty} dz_l V_{\text{int}}(z_l + x_m) \right] \\ &\times \frac{1}{\sqrt{(2\pi)^{n+1} \det a^2}} \exp \left(-\frac{1}{2} \sum_{k,l=0}^n z_k a_{kl}^{-2} z_l \right), \quad (13) \end{aligned}$$

where a^2 is a symmetric square matrix of the order of $(n+1)$. Its elements are obtained from the $G^{\Omega, p}(\tau, \tau')$ periodic Green functions of the harmonic oscillator [16,17]:

$$a^2(\tau, \tau') \equiv \frac{\hbar}{M} G^{\Omega, p}(\tau, \tau') = \frac{\hbar}{2M\Omega} \frac{\cosh(\Omega(|\tau - \tau'| - \hbar\beta/2))}{\sinh(\hbar\beta\Omega/2)} \quad (14)$$

and it represents the width of the fluctuations.

$\tilde{\rho}(x_b, x_a)$ can be written as a truncated series of the order of N , in terms of the cumulant functions $\langle A_{\text{int}}^n [x] \rangle_{x_b, x_a, c}^{\Omega, x_m}$.

$$\tilde{\rho}_N(x_b, x_a) = \tilde{\rho}_0(x_b, x_a) \exp \left[\sum_{n=1}^N \frac{(-1)^n}{n! \hbar^n} \langle A_{\text{int}}^n [x] \rangle_{x_b, x_a, c}^{\Omega, x_m} \right], \quad (15)$$

where $\langle A_{\text{int}}^n [x] \rangle_{x_b, x_a, c}^{\Omega, x_m}$ is given by:

$$\left\langle A_{\text{int}}^n [x] \right\rangle_{x_b, x_a, c}^{\Omega, x_m} = \langle A_{\text{int}}^n [x] \rangle_{x_a, x_a}^{\Omega} - \left(\left\langle A_{\text{int}} [x] \right\rangle_{x_a, x_a}^{\Omega} \right)^n. \quad (16)$$

The above expression depends explicitly on the two parameters Ω and x_m . Using the analogy with classical statistical physics,

$$\tilde{\rho}_{\text{cl}}(x) = (2\pi\hbar^2\beta/M)^{1/2} \exp[-\beta V(x)] \quad (17)$$

we can write a similar expression for $\tilde{\rho}(x_b, x_a)$:

$$\tilde{\rho}(x_b, x_a) = (2\pi\hbar^2\beta/M)^{1/2} \exp[-\beta V_{\text{eff,cl}}(x)] \quad (18)$$

we can then obtain the N -th order approximation of the potential $V_{\text{eff,cl}}$ from equations (14) and (17)

$$\begin{aligned} W_N^{\Omega, x_m} &= \frac{1}{2\beta} \ln \left(\frac{\sinh(\hbar\beta\Omega)}{\hbar\beta\Omega} \right) - \frac{1}{\beta} \sum_{n=1}^N \frac{(-1)^n}{n! \hbar^n} \langle A_{\text{int}}^n [x] \rangle_{x_b, x_a, c}^{\Omega, x_m} \\ &+ \frac{M\Omega}{2\hbar\beta \sinh(\hbar\beta\Omega)} \{ (\tilde{x}_b^2 + \tilde{x}_a^2) \coth(\hbar\beta\Omega) - 2\tilde{x}_b\tilde{x}_a \} \quad (19) \end{aligned}$$

with

$$\tilde{x}(\tau) = x(\tau) - x_m. \quad (20)$$

Optimisation of $W_N^{\Omega, x_m}(x_b, x_a)$ against Ω^2 and x_m

$$\frac{\partial W_N^{\Omega, x_m}(x_b, x_a)}{\partial \Omega^2} = 0 \quad \text{and} \quad \frac{\partial W_N^{\Omega, x_m}(x_b, x_a)}{\partial x_m} = 0$$

leads to the optimal values Ω_{opt}^2 and $x_{m \text{opt}}$. They give us the best approximation for $V_{\text{eff,cl}}(x_0)$ and lead to a good evaluation of the ground-state energy.

3. The ground-state energy for three particles subjected to a complex PT potential

The many-body problem occurs in several physical situations and the least difficult example is the three-body problem [18–20]. Let us consider the problem of three particles subjected to a complex PT potential. It was shown on the basis of numerical studies that the energy of such potentials is real and positive [1–13]. Note that the parity operator acts as P: $p \rightarrow -p$ and P: $x \rightarrow -x$, and that the antiunitarity time reversal operator acts as T: $p \rightarrow -p$, T: $x \rightarrow -x$ and T: $i \rightarrow -i$.

In our case, we consider the family of potentials given by:

$$\begin{aligned} V(x_1, x_2, x_3) = & A_1[(x_2 - x_3) + (x_1 - x_3)]^2 + A_2(x_2 - x_1)^2 \\ & \times A_5(x_2 - x_1)^{4m} + iA_3(x_2 - x_1)^{2m-1} + iA_4(x_2 - x_1)^{2m+1} \end{aligned} \quad (21)$$

where m is a positive parameter.

If we use the center-of-mass and Jacobi coordinates,

$$\begin{aligned} R &= \frac{1}{3}(x_1 + x_2 + x_3), \\ x &= \frac{1}{\sqrt{2}}(x_1 - x_2), \\ y &= \frac{1}{\sqrt{6}}(x_1 + x_2 - 2x_3), \end{aligned}$$

this potential becomes

$$V(x, y) = 6A_1y^2 + 2A_2x^2 + iB_3x^{2m-1} + iB_4x^{2m+1} + B_5x^{4m}, \quad (22)$$

where $B_3 = A_32^{m-1/2}$, $B_4 = A_42^{m+1/2}$ and $B_5 = A_52^m$.

The corresponding ground state energy is given by the following relation:

$$E_0 = \sqrt{3A_1} + E_{0x}.$$

The term E_{0x} is related to the x coordinate potential,

$$V(x) = 2A_2x^2 + iB_3x^{2m-1} + iB_4x^{2m+1} + B_5x^{4m}. \quad (23)$$

A study of the case $m = 1$, will allow us to obtain with a very good accuracy the complex PT potential ground state energy, and confirm that it is effectively real and positive. Hence, by setting $m = 1$, the potential $V(x)$ becomes:

$$V(x) = 2A_2x^2 + iB_3x + iB_4x^3 + B_5x^4. \quad (24)$$

By setting $\hbar = M = 1$, the corrected F-K method leads to a second order approximation of the classical effective potential $W_N^{\Omega, x_m}(x_b, x_a)$:

$$\begin{aligned} W_2^{\Omega, x_m}(x_b, x_a) = & \frac{1}{2\beta} \ln \left(\frac{\sinh(\hbar\beta\Omega)}{\hbar\beta\Omega} \right) + \frac{\Omega}{\beta \sinh(\hbar\beta\Omega)} x_a^2 \tanh(\beta\Omega/2) \\ & + \frac{1}{\beta} \left\langle A_{\text{int}}[x] \right\rangle_{x_a, x_a}^{\Omega} - \frac{1}{2\beta} \left\langle A_{\text{int}}^2[x] \right\rangle_{x_b, x_a, c}^{\Omega}, \end{aligned} \quad (25)$$

where

$$\left\langle A_{\text{int}}^2[x] \right\rangle_{x_b, x_a, c}^{\Omega, x_m} = \left\langle A_{\text{int}}^2[x] \right\rangle_{x_a, x_a}^{\Omega} - \left(\left\langle A_{\text{int}}[x] \right\rangle_{x_a, x_a}^{\Omega} \right)^2, \quad (26)$$

and with

$$\left\langle A_{\text{int}}[x] \right\rangle_{x_b, x_a}^{\Omega} = \beta \left[\begin{array}{l} g_0 + (1/2) C_{\beta}^1 g_1 H_1(x) + (1/8) C_{\beta}^2 g_2 H_2(x) \\ + (1/48) C_{\beta}^3 g_3 H_3(x) + (1/384) C_{\beta}^4 g_4 H_4(x) \end{array} \right]. \quad (27)$$

$H_n(x)$ being the Hermite polynomial of degree n , and the g_n parameters are given by:

$$\begin{aligned} g_0 &= 2A_2a_{00}^4 + 2A_2x_m^2 + IB_3x_m + 3IB_4x_ma_{00}^4 + IB_4x_m^3 + 3B_5a_{00}^8, \\ &\quad + 6B_5x_m^2a_{00}^4 + B_5x_m^4 - (1/2)\Omega^2a_{00}^4, \\ g_1 &= 3I\sqrt{2}B_4a_{00}^6 + 12\sqrt{2}B_5x_ma_{00}^6 + 4\sqrt{2}A_2x_ma_{00}^2 + I\sqrt{2}B_3a_{00}^2, \\ &\quad + 3I\sqrt{2}B_4x_m^2a_{00}^2 + 4\sqrt{2}B_5x_m^3a_{00}^2, \\ g_2 &= 24B_5a_{00}^8 + 8A_2a_{00}^2 + 12IB_4x_ma_{00}^4 - 2\Omega^2a_{00}^4 + 24B_5x_m^2a_{00}^2, \\ g_3 &= 12I\sqrt{2}B_4a_{00}^6 + 48\sqrt{2}B_5x_ma_{00}^6, \\ g_4 &= 96B_5a_{00}^8, \end{aligned}$$

the C_{β}^n are

$$C_{\beta}^n = \frac{1}{2^n \cosh^n(\beta\Omega/2)} \sum_{k=1}^N C_k^n \frac{\sinh(\beta\Omega(n/2 - k))}{\beta\Omega(n/2 - k)}, \quad (28)$$

at low temperature ($\beta \rightarrow \infty$), the coefficients C_β^n become:

$$\lim_{\beta \rightarrow \infty} C_\beta^n = \begin{cases} 1 & n = 0. \\ \frac{2}{n\beta\Omega} & n \succ 0. \end{cases}$$

The calculation of $\langle A_{\text{int}}[x] \rangle_{x_b, x_a}^\Omega$ is relatively simple compared with that of $\langle A_{\text{int}}^2[x] \rangle_{x_b, x_a}^\Omega$. We obtain:

$$\begin{aligned} \langle A_{\text{int}}^2[x] \rangle_{x_b, x_a}^\Omega &= \int_0^{h\beta} d\tau_1 \int_0^{h\beta} d\tau_2 \{ A^2 [I_{22}(\tau_1, \tau_2) - I_2(\tau_1) I_2(\tau_2)] \\ &\quad - B_3^2 [I_{11}(\tau_1, \tau_2) - I_1(\tau_1) I_1(\tau_2)] - B_4^2 [I_{33}(\tau_1, \tau_2) - I_3(\tau_1) I_3(\tau_2)] \\ &\quad + B_5^2 [I_{44}(\tau_1, \tau_2) - I_4(\tau_1) I_4(\tau_2)] - 2B_3 B_4 [I_{13}(\tau_1, \tau_2) - I_1(\tau_1) I_3(\tau_2)] \\ &\quad + 2IAB_4 [I_{23}(\tau_1, \tau_2) - I_2(\tau_1) I_3(\tau_2)] + 2IB_3 B_5 [I_{14}(\tau_1, \tau_2) - I_1(\tau_1) I_4(\tau_2)] \\ &\quad + 2AB_5 [I_{24}(\tau_1, \tau_2) - I_2(\tau_1) I_4(\tau_2)] + 2IB_4 B_5 [I_{34}(\tau_1, \tau_2) - I_3(\tau_1) I_4(\tau_2)] \\ &\quad + 2IB_3 A [I_{12}(\tau_1, \tau_2) - I_1(\tau_1) I_2(\tau_2)] \}. \end{aligned} \quad (29)$$

The $A(3, 3)$ square matrix, the $I_m(\tau_k)$ and $I_{mn}(\tau_1, \tau_2)$ terms appearing in (28) are given by:

$$\begin{aligned} A &= \frac{1}{2} (4A_2 - \Omega^2), \\ I_m(\tau_k) &= (a_{00}^4 - a_{0k}^4)^m \frac{\partial^m}{\partial j^m} \exp \left[\frac{j^2 + 2x_a a_{0k} j}{2a_{00}^2 (a_{00}^4 - a_{0k}^4)} \right]_{j=0}, \quad k = 1 \text{ and } 2, \end{aligned} \quad (30)$$

and

$$I_{mn}(\tau_1, \tau_2) = (-\det D)^{m+n} \frac{\partial^m}{\partial j_1^m} \frac{\partial^n}{\partial j_2^n} \exp \left[\frac{F(j_1, j_2)}{2a_{00}^2 \det(a^2)} \right]_{j_1=j_2=0} \quad (31)$$

$$\text{with } \det(a^2) = a_{00}^6 + 2a_{01}^2 a_{02}^2 a_{12}^2 - a_{00}^2 (a_{01}^4 + a_{02}^4 + a_{12}^4).$$

Moreover, the generating function $F(j_1, j_2)$ is given by:

$$\begin{aligned} F(j_1, j_2) &= a_{00}^4 (j_1^2 + j_2^2) - 2a_{00}^6 (a_{01}^2 j_1 + a_{02}^2 j_2) x_a \\ &\quad + 2a_{00}^2 (a_{12}^2 j_1 j_2 + (a_{01}^4 + a_{02}^4 + a_{12}^4) (a_{01}^2 j_1 + a_{02}^2 j_2) x_a) \\ &\quad - (a_{01}^2 j_1 + a_{02}^2 j_2) (a_{01}^2 j_1 + a_{02}^2 j_2 + 4a_{01}^2 a_{02}^2 a_{12}^2 x_a). \end{aligned} \quad (32)$$

The calculation of $W_2^\Omega(x_a)$ allows us to get successively, the particles density $\tilde{\rho}_2^\Omega(x_a)$, the partition function Z_2 and the ground-state energy E_0 :

$$\tilde{\rho}_2^\Omega(x_a) = \frac{1}{\sqrt{2\pi\beta}} \exp[-\beta W_2^\Omega(x_a)], \quad (33)$$

$$Z_2 = \int dx_a \tilde{\rho}_2^\Omega(x_a), \quad (34)$$

and

$$E_0 = \lim_{\beta \rightarrow \infty} \left(-\frac{1}{\beta} \ln Z_2 \right). \quad (35)$$

4. Results and discussions

The ground state energy of a complex PT potential (20) has been calculated by the corrected F–K variational method, using different sets of the A_i parameters. The obtained results (see Table I) are compared with those exactly calculated via the QES potentials method [21–24]. Note that, the aforesaid method allows us to obtain exact energies by imposing constraints on the parameters of the studied potential.

Our results are in a good agreement with the exact ones. This can be explained by the fact that the corrections introduced in this work, have a strong influence on the effective potential W_N^{Ω, x_m} and consequently on the ground state energy E_0 at low temperatures. Indeed, the variation ΔE_0 is proportional to $\Delta W_N^{\Omega, x_m}$. Besides, the same effects have a much greater influence on the particle density $\rho(x)$ and the partition function Z , where their variations $\Delta \rho$ and ΔZ are the exponential function of $\Delta W_N^{\Omega, x_m}$

$$\Delta \rho \sim \exp(-\beta \Delta W_N^{\Omega}) \quad \text{and} \quad \Delta Z \sim \exp(-\beta \Delta W_N^{\Omega}).$$

TABLE I

Ground state energy for potential (21) with different values of the A_i parameters.

A_1	A_2	A_3	A_4	E_{method}	E_{QES}
0.05	0.2	−0.031623	−0.00125	0.313122	0.31623
0.01	1	−0.01414	−0.00005	0.702614	0.70711
0.5	5	−1.58114	−0.125	1.568689	1.58114
3	10	−13.41641	−4.5	2.208198	2.23606
10	10^3	−447.2136	−50	22.34119	22.3606
30	10^4	−4242.6407	−450	70.69306	70.71068
200	10^5	−89442.72	−2.10 ⁴	223.5310	223.6068

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