

PHHQP XI: Non-Hermitian Operators in Quantum Physics  
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**The variational perturbation method  
applied to a family of anharmonic  
complex-PT potentials**

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# Plan

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- Introduction.
- Brief overview on Feynman-Kleinert variational method.
- Application.
- Building a complex - PT potential from the Q.E.S method.
- Results and discussions.
- Conclusion.

# 1.Introduction

Methods of  
calculation

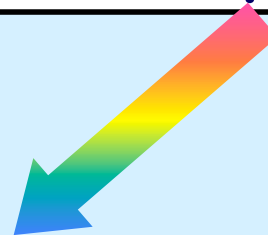


Schrödinger's equation  
associated to a given physical  
system

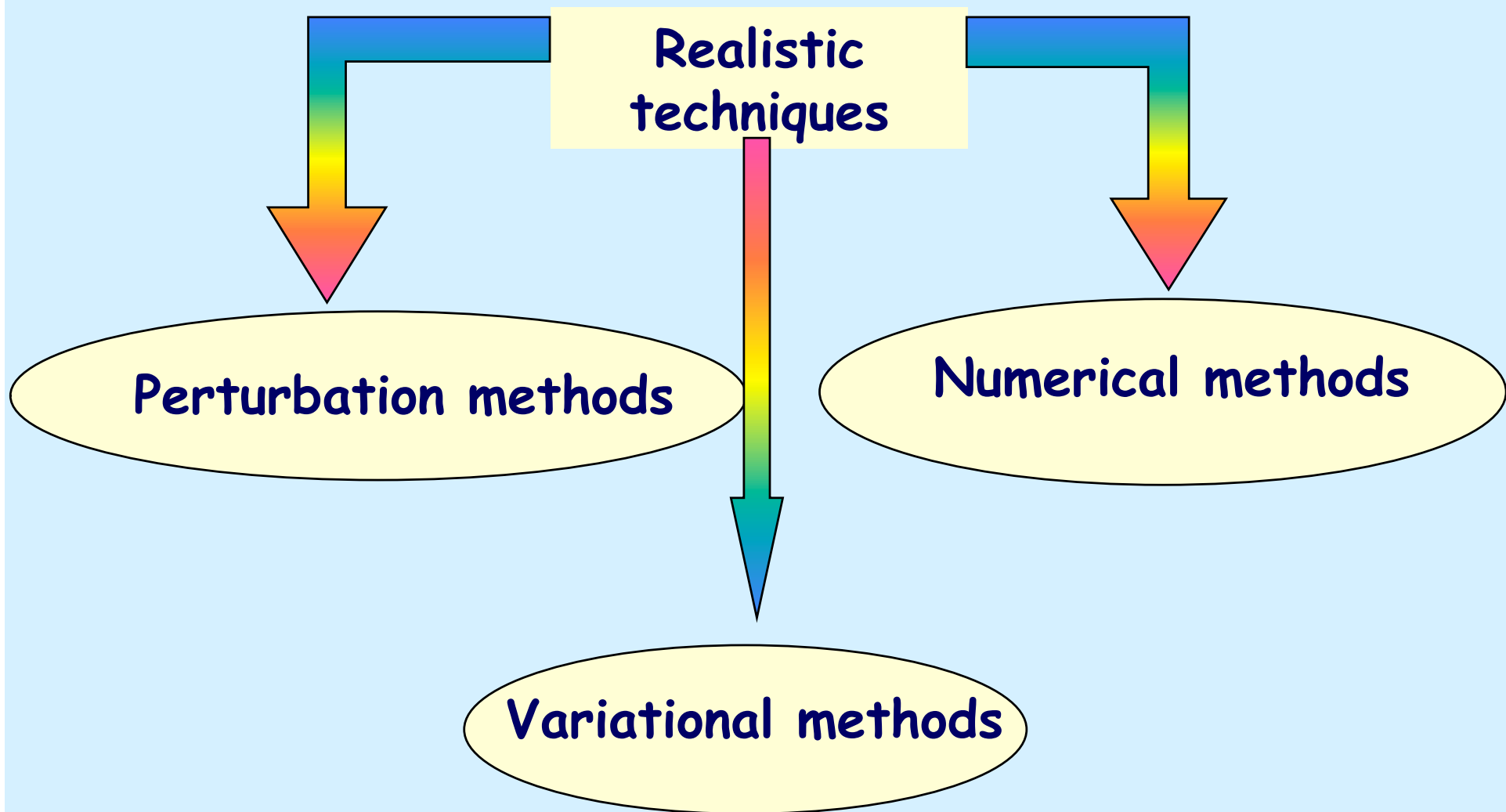
Most cases



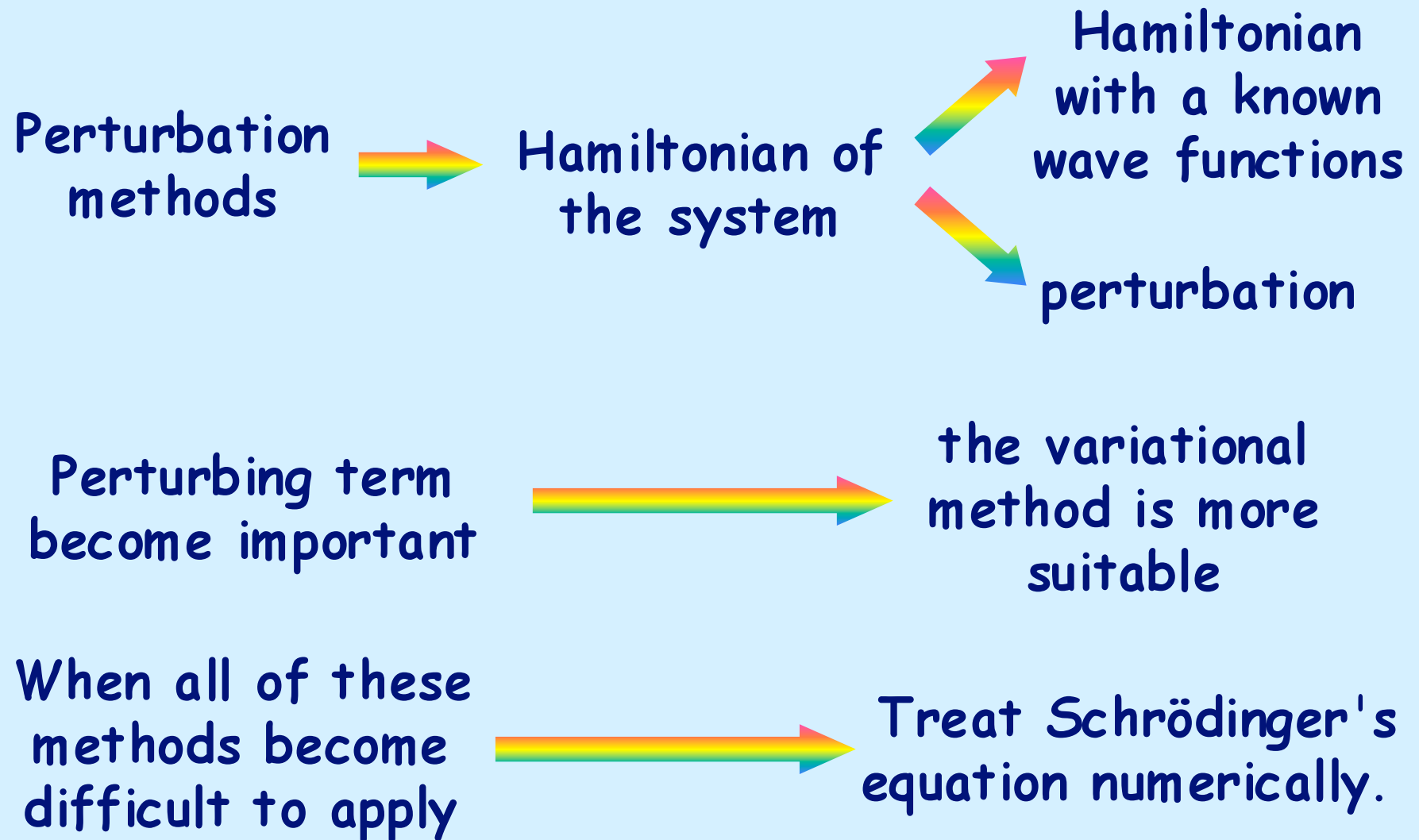
Techniques based on exact  
calculation proved to be unsuited  
to solve problems where potentials  
are complicated.



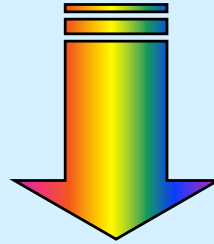
We use generally realistic  
techniques to approach the studied  
system.



# 1.Introduction



**Feynman formalism**



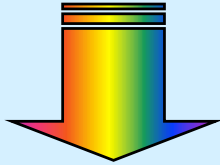
**An integral formulation of quantum mechanics**

## First applications

- Simple cases have been exactly calculated:
  - Free particle.
  - Harmonic oscillator.
  - Physical systems described by quadratic Lagrangians.
- ➡ New techniques like a coordinates transformation  $x \rightarrow f(q)$  followed by temporal transformation  $t \rightarrow s$  have been developed in order to extend the formalism to less simple cases.

# Feynman formalism

Variational method  
called Feynman-  
Kleinert method



Kleinert has  
introduced some  
improvements in the  
F-K method

some formal similarities



Ritz method



Variational  
perturbation method

➤ based on the density matrix development on the basis of the harmonic oscillator wave functions, and leads to acceptable results in the case of anharmonic potentials.



## II. Brief overview on Feynman-Kleinert variational method

The partition function calculation is reduced to that of effective classical partition function using a trial harmonic potential of pulsation  $\Omega$ . In this approach, the partition function of particle moving into a potential  $V(x)$  is given by:

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

Where  $V_{\text{eff},cl}$  is the effective classical potential which takes into account all quantum effects, and  $x_0$  is the average position occupied by the particle in the temperature interval  $[0,\beta]$ .

where  $\beta=1/k_bT$ ,  $k_b$  is the Boltzmann constant.

## II. Brief overview on Feynman-Kleinert variational method

$Z$  can be written

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

Where  $A[x]$  is the Euclidean action of the studied system.  
By identifying :

$$V_{eff,cl}(x_0) = -\frac{1}{\beta} \ln \left( \int \mathfrak{D}(x) \delta(\bar{x} - x_0) \exp \left[ -\frac{\mathcal{A}[x]}{\hbar} \right] \right)$$

It is possible to determine analytically  $V_{eff,cl}$  only for a very limited number of cases. So, we have to approximate the potential  $V_{eff,cl}(x_0)$  by the best potential  $W_N(x_0)$  obtained by a variational treatment. The  $N$ th order approximation of the partition function is given by:

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

## II. Brief overview on Feynman-Kleinert variational method

The potential  $V_{\text{eff},cl}$  is developed around the position  $x_0$ . The obtained series will be truncated at the order  $N$  and optimized versus  $\Omega$ , in order to obtain the best approximated  $W_N$

To apply this technique to the density matrix

$$\mathcal{A}[x] = \mathcal{A}^{\Omega, x_m}[x] + \mathcal{A}_{int}[x]$$

the trial action

the interaction

## II. Brief overview on Feynman-Kleinert variational method

The interaction is given by

$$\mathcal{A}_{int}[x] = \int_0^{\hbar\beta} V_{int}[x(\tau)] d\tau$$

with

$$V_{int}(x) = V(x) - \frac{M}{2}\Omega(x - x_m)^2$$

Let consider the density matrix defined as:

$$\tilde{\rho}(x_b, x_a) = \frac{1}{Z} \int_{(x_a, 0) \rightsquigarrow (x_b, \hbar\beta)} \mathfrak{D}(x) \exp \left[ -\frac{\mathcal{A}[x]}{\hbar} \right]$$

developing it in series of  $\mathcal{A}_{int}$

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

## II. Brief overview on Feynman-Kleinert variational method

The different terms appearing in the last equation have been already calculated by Kleinert, and they are given by

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

where  $a^2$  is a symmetric square matrix of order  $(n+1)$ . Its elements are obtained from the periodic Green functions of the harmonic oscillator:

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

The density matrix can be written as a truncated series of order  $N$ , in terms of the cumulant functions

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

## II. Brief overview on Feynman-Kleinert variational method

Using the analogy with the classical statistical physics

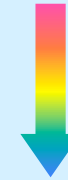


Classical statistical physics

Quantum statistical physics



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



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

The N order approximation of the potential  $V_{eff,cl}$  can be obtained from the expression of the last equation.

## II. Brief overview on Feynman-Kleinert variational method

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

Optimization with respect to  $\Omega^2$  and  $x_m$  leads to the resolution of the set of equations:

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

The optimal values of  $\Omega^2$  and  $x_m$  obtained allow us to achieve the best approximation to  $V_{\text{eff}, \text{cl}}$  and hence the energy of the ground state of the studied physical system.

### III. Application

The corrected F-K method has been already successfully applied to some forms of potentials as the Coulomb potential and the Double well potential.

- M. Bachman, H. Kleinert and A. Pelster, Phys. Rev, A V60 N°5 (1999) 3429.

- H. Kleinert , Path integrals in Quantum Mechanics, Statistics and Polymer Physics ( World scientific, Singapore, 2009).

- W. Janke, H. Kleinert, Phys. Rev. Lett. 75 (1995) 2787.

Application  Test its performances complex -PT potentials

$$V(x) = A_2 x^2 + i A_1 x + i A_3 x^3 + A_4 x^4$$



### III. Application

By setting  $\hbar=M=1$ , the previous technique leads, for the studied potential, to a second order approximation of the classical effective potential

$$W_2^{\Omega, x_m}(x_a) = \frac{1}{2\beta} \ln\left(\frac{\sinh(\hbar\beta\Omega)}{\hbar\beta\Omega}\right) + \frac{\Omega}{\beta \sinh(\hbar\beta\Omega)} x_a^2 \tanh(\beta\Omega/2) \\ + \frac{1}{\beta} \langle \mathcal{A}_{int}[x] \rangle_{x_a, x_a}^{\Omega} - \frac{1}{2\beta} \langle \mathcal{A}_{int}^2[x] \rangle_{x_a, x_a, c}^{\Omega}$$

where

$$\langle \mathcal{A}_{int}^2[x] \rangle_{x_a, x_a, c}^{\Omega, x_m} = \langle \mathcal{A}_{int}^2[x] \rangle_{x_a, x_a}^{\Omega} - (\langle \mathcal{A}_{int}[x] \rangle_{x_a, x_a}^{\Omega})^2$$

with

$$\langle \mathcal{A}_{int}[x] \rangle_{x_a, x_a}^{\Omega} = \beta[g_0 + (1./2.)C_{\beta}^1 g_1 H_1(x) + (1./8.)g_2 H_2(x)C_{\beta}^2 \\ + (1./48.)g_3 H_3(x)C_{\beta}^3 + (1./384.)g_4 H_4(x)C_{\beta}^4]$$

### III. Application

Where  $H_n(x)$  is the hermite polynomial of degree  $n$ , and the  $g_i$  parameters are given by:

$$g_0 = A_2 a_{00}^4 + A_2 x_m^2 + I A_1 x_m + 3 I A_3 x_m a_{00}^4 + I A_3 x_m^3 + 3 A_4 a_{00}^8 + 6 A_4 x_m^2 a_{00}^4 + A_4 x_m^4 - (1/2) \Omega^2 a_{00}^4$$

$$g_1 = 3 I \sqrt{2} a_{00}^6 A_3 + 12 \sqrt{2} a_{00}^6 A_4 x_m + 2 \sqrt{2} a_{00}^2 A_2 x_m + I \sqrt{2} a_{00}^2 A_1 + 3 I \sqrt{2} a_{00}^2 A_3 x_m^2 + 4 \sqrt{2} a_{00}^2 A_4 x_m^3$$

$$g_2 = 24 a_{00}^8 A_4 + 4 A_2 a_{00}^2 + 12 I A_3 x_m a_{00}^4 - 2 \Omega^2 a_{00}^4 + 24 A_4 x_m^2 a_{00}^2$$

$$g_3 = 12 I \sqrt{2} a_{00}^6 A_3 + 48 \sqrt{2} a_{00}^6 A_4 x_m$$

$$g_4 = 96 A_4 a_{00}^8$$

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

### III. Application

$$\begin{aligned}
 \langle \mathcal{A}_{int}^2[x] \rangle_{x_a, x_a}^\Omega &= \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \{ A^2 [I_{22}(\tau_1, \tau_2) - I_2(\tau_1)I_2(\tau_2)] - A_1^2 [I_{11}(\tau_1, \tau_2) - I_1(\tau_1)I_1(\tau_2)] \\
 &\quad - A_3^2 [I_{33}(\tau_1, \tau_2) - I_3(\tau_1)I_3(\tau_2)] + A_4^2 [I_{44}(\tau_1, \tau_2) - I_4(\tau_1)I_4(\tau_2)] \\
 &\quad - 2A_1A_3 [I_{13}(\tau_1, \tau_2) - I_1(\tau_1)I_3(\tau_2)] + 2IAA_3 [I_{23}(\tau_1, \tau_2) - I_2(\tau_1)I_3(\tau_2)] \\
 &\quad + 2IA_1A_4 [I_{14}(\tau_1, \tau_2) - I_1(\tau_1)I_4(\tau_2)] + 2AA_4 [I_{24}(\tau_1, \tau_2) - I_2(\tau_1)I_4(\tau_2)] \\
 &\quad + 2IA_3A_4 [I_{34}(\tau_1, \tau_2) - I_3(\tau_1)I_4(\tau_2)] + 2IA_1A [I_{12}(\tau_1, \tau_2) - I_1(\tau_1)I_2(\tau_2)] \}
 \end{aligned}$$

the quantity  $W_2^{\Omega, x_m}(x_a)$  allows us to get successively, the particles density, the partition function and the ground state energy via the relations :

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

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

$$E_K = \lim_{\beta \rightarrow \infty} \left( -\frac{1}{\beta} \ln Z_2 \right)$$

## IV. Building a complex - PT potential from the Q.E.S method

To test the performance of the method



we need to an exact ground state energy



The Quasi Exactly Solved potentials method

Let us choose a test function



$$\Psi_n(x) = x^n \exp(-\alpha x^2 + i\beta x^3)$$

Derivation leads to

$$-\frac{1}{2}\Psi''_n(x) = \left[\frac{n(1-n)}{2x^2} + (2n\alpha + \alpha) - 3i\beta(1+n)x - 2\alpha^2 x^2 + 6i\alpha\beta x^3 + \frac{9}{2}\beta^2 x^4\right]\Psi_n(x)$$

## IV. Building a complex - PT potential from the Q.E.S method

Comparison with

$$-\frac{1}{2}\Psi''_n(x) = [E - V(x)]\Psi_n(x)$$

gives

$$E_n = (2n + 1)\alpha$$
$$A_1 = 3\beta, A_2 = 2\alpha^2, A_3 = -6\alpha\beta \text{ and } A_4 = -\frac{9}{2}\beta^2$$

The energy spectrum is real and positive.

## IV. Results and discussions:

The general form

$$V(x) = A_2x^2 + iA_1x + iA_3x^3 + A_4x^4$$

$A_2$	$A_1$	$A_3$	$A_4$	$E_{method}$	$E_{QES}$
3.4848	0.3	-0.792	-0.045	1.319	1.32
8	3	-12	-4.5	1.956	2
0.02	0.03	-0.006	-0.00045	0.099	0.1
0.5	0.003	-0.003	$-0.45 \cdot 10^{-5}$	0.4995	0.5
50	9	-90	-45.5	4.973	5
200	3	-60	-4.5	9.999	10
$5 \cdot 10^{-2}$	0.3	-0.03	-0.045	-0.856	0.05
800	15	-600	-112.5	19.999	20
2	15	-30	-112.5	-658.602	1
$2 \cdot 10^4$	6	-1200	-18	99.999	100
$2 \cdot 10^6$	150	$-3 \cdot 10^5$	-11250	999.999	1000

$E_{method}$

Our calculations

$E_{QES}$

The Quasi Exactly Solved potentials method

## The first special case : $A_1=A_4=0$

$$V(x) = A_2x^2 + iA_3x^3$$

$A_2$	$A_3$	$E_{method}$	$E_{num}$
0.5	0.03125	0.50276	0.50263
0.5	0.06250	0.50621	0.50998
0.5	0.1250	0.51964	0.53393
0.5	0.25	0.58522	0.59492
0.5	0.5	0.73773	0.71294

$E_{method}$  Our calculations

$E_{num}$  C. M. Bender, G. Dunne, Phys. Rev.A, V40 N°10 (1999)  
4616.

## The second special case : $A_3=A_4=0$

$$V(x) = A_2x^2 + iA_1x$$

$A_2$	$A_1$	$E_{method}$	$E_{exact}$
0.1	0.01	0.2234017	0.2238567
0.5	0.01	0.4995548	0.5000050
1.	0.1	0.7091212	0.7096067
5.	0.1	1.5849085	1.5816388
10.	1.	2.2607512	2.2610679
100.	1.	7.0976602	7.0705678

$E_{method}$  Our calculations

$E_{exact}$  Exact treatment



**The third special case :  $A_3=A_1=0$ .**

$$V(x) = A_2x^2 + A_4x^4$$

$A_2$	$A_4$	$E_{method}$	$E_{exact}$
0.5	0.025	0.545205	0.559146
0.5	0.05	0.589395	0.602405
0.5	0.075	0.607374	0.637992
0.5	0.1	0.612889	0.668773
0.5	0.125	0.607404	0.696176
0.5	0.15	0.599178	0.721039
0.5	0.175	0.580685	0.743904

$E_{method}$  **Our calculations**

$E_{exact}$  **H. Kleinert, Phys. Lett. A 173 (1993) 332.**

## Conclusion

- Calculation by the corrected Feynman-Kleinert variational method, of the energy ground state of the PT-symmetric complex potential by considering various sets of potential parameters.
- The results are compared later to those calculated exactly by the QES potential method.
- Our results compare favorably with exact results.

## Conclusion

- We noticed that for very large values of  $\beta$  to those of  $\alpha$ , the gap is not insignificant and the method leads to unsatisfactory results. This is explained by the fact that in such cases, the wave function describes a double well potential that deviates from the harmonic oscillator.
- We also considered three special cases of the studied potential.

# Perspectives

- Extend the corrected Feynman-Kleinert approximation method to calculate the ground state energy of a PT-symmetric complex potential of order 6.
- The family of potentials contains various orders of anharmonicity, which allows him to include several families of phenomenological potential used in physics.

**Thank you for  
your attention**