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Improving the variational path integral approach to the quantum double-well potential

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Abstract

An improved variational path integral approach is developed and applied to the quantum double-well potential, in which part of the quartic term of the potential is included in the trial action. The expression of the effective classical potential (ECP) under a non-Gaussian expectation is obtained. Here the frequency and fourth-order derivative of the potential are treated as two variational parameters, determined by the minimization of the ECP at each point. We calculate the ECP, the free energy and the level splitting of a symmetrical double-well potential. It is shown that the present results are better than those of the Feynman–Kleinert Gaussian variational method.

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1. Introduction

Feynman proposed the well-known effective classical potential (ECP) approach to calculate the partition function of a quantum system described by the path integrals in his two textbooks [1, 2]. The starting point is that the exponentiation of the kinetic action is regarded as a Gaussian distribution and the path integrals are converted into a one-dimensional averaging under this distribution. Jensen's inequality in the probability theory is applied to the functional integrals and an upper bound for the free energy is found. A considerable improvement on Feynman's original variational method has been proposed by Giachetti and Tognetti [3], and independently by Feynman and Kleinert (F–K) [4]. The basic idea is to combine the quadratic term of the potential and the kinetic energy to make a quadratic trial action. Then the oscillator frequency of the potential is considered to be a variational parameter and is determined by the minimization of the ECP. In fact, the F–K variational path integral method can be understood to involve analytically most information in the trial action, and the remaining action

is decreased as much as possible. Some reviews can be found in the books by Kleinert [5] and Weiss [6].

Recently, Kleinert and his collaborators have developed a third-order perturbation expansion to improve the accuracy of the problems of the anharmonic oscillator [7–9]. They expanded the action into a perturbation series and did not use the Jensen's inequality, the higher-order approximation for the ECP was iterated. The results obtained are more accurate than the F–K approach. However, it is still based on the Gaussian expectation technique. This method could cause a divergent difficulty when one applies it to a multi-stable potential [10] or a nonlinear dissipative system [11–13] near the crossover temperature [10].

Moreover, the accuracy of the variational path integral approach can be checked by the effective oscillator frequency of the ECP; i.e. when the temperature is lowered, the effective oscillator frequency at the bottom of the potential well will converge to the difference between the second and first quantal energy levels. For the anharmonic potential, the procedures are very good. But, if the method is applied to the double-well potential with a high barrier, the variational result diverges greatly from the exact value of quantum mechanics [14]. Indeed, the usual variational path integral method uses the Gaussian smeared procedure. At low temperature, the eigenvalues of the low-order fluctuation models will approach zero, thus the corresponding integrals diverge [6, 10]. The effective oscillator frequency in the F–K method is much larger than the realistic frequency.

In this paper, we generalize the Gaussian measure to the non-Gaussian measure consisting of part of the quadric term of the potential, and we introduce a new trial action with two variational parameters. Thus, the remaining action arrives at a local minimum for a double-well potential. We compare the non-Gaussian measurement technique with the F–K method for the double-well potential.

2. Approach

2.1. Fourth-order trial action

In Euclidean space, a quantum particle provides the centroid of its thermal path $x_0 = (\hbar\beta)^{-1}\int_0^{\hbar\beta} x(\tau)\,\mathrm{d}\tau$, where $x(\tau) = x_0 + x_1(\tau)$, $x_1(\tau)$ is the fluctuation part of the trajectory, β is the inverse temperature and τ is the imaginary time. The partition function of the system is written as a functional integral form [1–6]

$$Z = \int_{-\infty}^{\infty}\sqrt{\frac{m}{2\pi\hbar^2\beta}}\,\mathrm{d}x_0\oint D[x_1(\tau)]\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\left[\frac{1}{2}m\dot{x}(\tau)^2 + V(x(\tau))\right]\right\}. \tag{1}$$

The periodic paths with $x(0) = x(\hbar\beta)$ are now written as a Fourier decomposition, so that the paths and the functional integral measure have the following forms [5, 6]

$$\begin{aligned} x(\tau) &= x_0 + \sum_{n=-\infty, n\neq 0}^{\infty} X_n \exp(\mathrm{i}\theta_n\tau) \\ \oint D[x_1(\tau)] &= \prod_{n=1}^{\infty}\left[\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\beta m\theta_n^2}{\pi}\,\mathrm{d}\mathrm{Re}X_n\,\mathrm{d}\mathrm{Im}X_n\right] \end{aligned} \tag{2}$$

where $\theta_n = 2\pi n/\hbar\beta$ are the Matsubara frequencies. In order to have a real $x(\tau)$, we must require that $X_n = X_{-n}^*$. It can easily be shown that the same measure is applicable to any system with the standard kinetic term [5, 6].

With the measure of integration (2), if one is able to perform the $n \neq 0$ integrals, this would leave Z as a one-dimensional integral

$$Z = \int_{-\infty}^{\infty} \sqrt{\frac{m}{2\pi\hbar^2\beta}}\, \mathrm{d}x_0 \exp[-\beta W(x_0)] \tag{3}$$

where $W(x_0)$ is called the ECP. This agrees with the classical statistical partition function when the temperature $T \to \infty$.

In this paper, we consider a symmetrical double-well potential

$$V(x) = -\tfrac{1}{2}x^2 + \tfrac{1}{4}gx^4 \tag{4}$$

where g is the coupling constant. We expand the potential into

$$V(x(\tau)) = \tfrac{1}{2}m\Omega^2(x_0)(x(\tau) - x_0)^2 + \tfrac{1}{4}mc_4(x_0)(x(\tau) - x_0)^4 + \tilde{V}(x(\tau)) \tag{5}$$

everywhere. Here, $\Omega^2(x_0)$ and $c_4(x_0)$ are two x_0-dependent variational parameters.

Substituting equations (2) and (5) into equation (1), we yield a fourth-order trial action

$$S = \sum_{n=1}^{\infty} \hbar\beta m \left[\theta_n^2 + \Omega^2(x_0)\right] X_n X_{-n} + \frac{3}{2}\sum_{n=1}^{\infty} \hbar\beta m c_4(x_0) X_n^2 X_{-n}^2 + S_{\mathrm{rem}} \tag{6}$$

where the remaining part of the action is given by

$$S_{\mathrm{rem}} = \int_0^{\hbar\beta} V(x(\tau))\, \mathrm{d}\tau - \hbar\beta m\Omega^2(x_0) \sum_{n=1}^{\infty} X_n X_{-n} - \frac{3}{2}\hbar\beta m c_4(x_0) \sum_{n=1}^{\infty} X_n^2 X_{-n}^2. \tag{7}$$

Then equation (3) can be expressed by an averaging under a non-Gaussian distribution, i.e.

$$\begin{aligned}\exp[-\beta W(x_0)] &= \oint D[x_1(\tau)] \exp\left\{-m\beta \sum_{n=1}^{\infty} A_n X_n X_{-n}\right. \\ &\quad \left. - m\beta \sum_{n=1}^{\infty} B X_n^2 X_{-n}^2 \right\} \exp\left(-\frac{1}{\hbar} S_{\mathrm{rem}}[x(\tau)]\right) \\ &= Z_1(x_0) \left\langle \exp\left(-\frac{1}{\hbar} S_{\mathrm{rem}}\right)\right\rangle_2 \end{aligned} \tag{8}$$

with

$$\begin{aligned} Z_1 &= \prod_{n=1}^{\infty} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\beta m\theta_n^2}{\pi}\, \mathrm{dRe}X_n\, \mathrm{dIm}X_n \cdot \exp\left[-m\beta \sum_{n=1}^{\infty} \left(A_n X_n X_{-n} + B X_n^2 X_{-n}^2\right)\right] \\ &= \prod_{n=1}^{\infty} I_n \theta_n^2. \end{aligned} \tag{9}$$

Here, $A_n = \theta_n^2 + \Omega^2(x_0)$, $B = \frac{3}{2}c_4(x_0)$,

$$I_n = \sqrt{\frac{\pi m\beta}{4B}}\, \mathrm{erfc}\left(A_n \sqrt{\frac{m\beta}{4B}}\right) \exp\left(A_n^2 \frac{m\beta}{4B}\right) \tag{10}$$

as well as the bracket $\langle \cdots \rangle_2$ indicate the averaging under the following normalized non-Gaussian distribution:

$$Z_1^{-1} \exp\left\{-m\beta \sum_{n=1}^{\infty} \left(A_n X_n X_{-n} + B X_n^2 X_{-n}^2\right)\right\}. \tag{11}$$

If $\Omega^2(x_0) < 0$, the value of A_n could be equal to zero. The expectation of the thermodynamical functions should diverge in the F–K method with $B = 0$ [4, 5] and then

$I_n^{-1} \to A_n$. Because B is positive for a bound potential in general, the value of I_n will remain finite while $A_n \to 0$, thus the statistical average of any physical quantity under distribution (11) always exists.

To optimize the effective partition function, we apply Jensen's inequality, $\langle \exp(-F)\rangle \geqslant \exp(-\langle F\rangle)$, to equation (8), namely,

$$\exp[-\beta W(x_0)] \geqslant \exp[-\beta W_1(x_0)] = Z_1 \exp\left\{-\frac{1}{\hbar}\left\langle \int_0^{\hbar\beta}\left[V(x(\tau)) - \frac{1}{2}m\Omega^2(x_0)(x(\tau)-x_0)^2\right]\mathrm{d}\tau - \frac{3}{2}\hbar\beta m c_4(x_0)\sum_{n=1}^{\infty} X_n^2 X_{-n}^2\right\rangle_2\right\}. \tag{12}$$

This leads to a bounded $W(x_0)$ by $W_1(x_0)$ from above, $W(x_0) \leqslant W_1(x_0)$.

2.2. Non-Gaussian expectation

The average of the double-well potential $V(x(\tau))$ under distribution (11) can be found exactly. For example, it is straightforward to calculate the integral of the fourth moment of the coordinate

$$\frac{1}{\hbar\beta}\left\langle \int_0^{\hbar\beta} x(\tau)^4 \mathrm{d}\tau\right\rangle_2 = \left\langle x_0^4\right\rangle_2 + 6x_0^2\sum_{n=1}^{\infty} 2\langle X_n X_{-n}\rangle_2 + 6\sum_{n=1}^{\infty}\left\langle X_n^2 X_{-n}^2\right\rangle_2 + 3\left\{\left(\sum_{n=1}^{\infty}\langle 2X_n X_{-n}\rangle_2\right)^2 - \sum_{n=1}^{\infty} 4(\langle X_n X_{-n}\rangle_2)^2\right\}. \tag{13}$$

Then we obtain the expectation of the remaining action

$$\frac{1}{\hbar\beta}\langle S\mathrm{rem}\rangle_2 = -\frac{1}{2}x_0^2 + \frac{1}{4}gx_0^4 + \frac{1}{2}\left(3gx_0^2 - m\Omega^2 - 1\right)\sum_{n=1}^{\infty} 2\langle X_n X_{-n}\rangle_2 + \frac{3}{4}(g - mc_4)\sum_{n=1}^{\infty} 2\left\langle X_n^2 X_{-n}^2\right\rangle_2 + \frac{3}{4}g\left[\left(\sum_{n=1}^{\infty}\langle 2X_n X_{-n}\rangle_2\right)^2 - \sum_{n=1}^{\infty} 4(\langle X_n X_{-n}\rangle_2)^2\right].$$

The ECP is finally obtained

$$W_1(x_0) = -\frac{1}{\beta}\sum_{n=1}^{\infty}\ln\left(\theta_n^2 I_n\right) + V_{a^2}(x_0) - \frac{1}{2}m\Omega^2(x_0)a^2(x_0) + \frac{3}{4}[g - mc_4(x_0)]\zeta(x_0) - \frac{3}{4}g\eta(x_0) \tag{14}$$

where the smeared potential of (4) in the above equation is given by

$$V_{a^2}(x_0) = -\tfrac{1}{2}x_0^2 + \tfrac{1}{4}gx_0^4 + \tfrac{1}{2}\left(3gx_0^2 - 1\right)a^2 + \tfrac{3}{4}ga^4 \tag{15}$$

and

$$a^2 = \sum_{n=1}^{\infty} 2\langle X_n X_{-n}\rangle_2 \qquad \zeta = \sum_{n=1}^{\infty} 2\left\langle X_n^2 X_{-n}^2\right\rangle_2 \qquad \eta = \sum_{n=1}^{\infty} 4\langle X_n X_{-n}\rangle_2^2. \tag{16}$$

Three quantities in equation (16) are evaluated from the integral I_n in the polar coordinate [6, 10], i.e.

$$\langle X_n X_{-n}\rangle_2 = -\frac{1}{m\beta}\frac{1}{I_n}\frac{\partial I_n}{\partial \Omega^2} \qquad \left\langle X_n^2 X_{-n}^2\right\rangle_2 = -\frac{1}{m\beta}\frac{1}{I_n}\frac{\partial I_n}{\partial B}. \tag{17}$$

Considering Ω^2 and c_4 as functions of x_0 which are calculated at each point x_0, we minimize $W_1(x_0, \Omega^2(x_0), c_4(x_0))$ with respect to the parameters $\Omega^2(x_0)$ and $B(x_0)$. Explicitly, the combined equations need to be solved numerically

$$\begin{aligned}
\frac{\partial W_1}{\partial \Omega^2} &= \frac{3}{4}g\frac{\partial}{\partial \Omega^2}(\zeta-\eta) - \frac{1}{2}mB\frac{\partial \zeta}{\partial \Omega^2} + \left(\frac{\partial V_{a^2}}{\partial a^2} - \frac{1}{2}m\Omega^2\right)\frac{\partial a^2}{\partial \Omega^2} = 0 \\
\frac{\partial W_1}{\partial B} &= \frac{3}{4}g\frac{\partial}{\partial B}(\zeta-\eta) - \frac{1}{2}mB\frac{\partial \zeta}{\partial B} + \left(\frac{\partial V_{a^2}}{\partial a^2} - \frac{1}{2}m\Omega^2\right)\frac{\partial a^2}{\partial B} = 0.
\end{aligned} \tag{18}$$

Indeed, the F–K quadratic variational method [4] is equivalent to our approach while $B = 0$, in this case, $\frac{\partial V_{a^2}}{\partial a^2} - \frac{1}{2}m\Omega^2 = 0$. However, here we have introduced a small positive parameter B; the derivative of $W_1(x_0)$ with regard to B is determined by the first term on the right-hand side of the second equation of (18). One can expand I_n into a power series of B as $B \to 0$

$$I_n = \frac{1}{A_n}\left(1 - \frac{2B}{m\beta A_n^2} + \frac{12B^2}{m^2\beta^2 A_n^4}\right) \tag{19}$$

so that

$$\zeta - \eta = -\frac{8}{m^3\beta^3}\sum_{n=1}^{\infty}\frac{B}{A_n^4} \tag{20}$$

is negative. Thus, it is concluded that the variation of c_4 will result in an accurate estimation for the ECP.

3. Results and discussion

In this paper, the natural units $\hbar = m = 1$ are used. We solve numerically the first equation for the variable Ω^2 in (18) for different c_4, where the value of c_4 is sought to yield the best lower limit of $W_1(x_0)$ at each point x_0.

In figure 1, the ECP of the double-well potential (4) with the coupling constant $g = 0.2$ is plotted for different temperatures and compared with the F–K method [4]. It is observed that our result is lower than that of the F–K method. Especially, when the temperature decreases and the coupling constant g becomes small, the difference between the present method and the F–K method is increased. It is noticed that there are new metastable points near the point $x_0 = 0$ when $\beta \geqslant 25$. This can be understood well from the point of view of quantum mechanics. It originates in a reiterative effect of two separate sets of oscillator wavefunctions. The detailed correction for the free energy is not very large, but may give rise to large effects on the problems related to the barrier dynamics and tunnelling.

In figure 2, we calculate the free energy $F = -\frac{1}{\beta}\ln Z$ as a function of the inverse temperature using our procedure and the F–K method. Because the main contribution of the free energy comes from the bottom of the potential well, where the effect of the negative oscillator frequency of the trial potential is weak, thus the correction to the free energy is not easily observed. However, the effects of the fourth-order term of the potential cannot be ignored for $\beta > 5$.

In figure 3, the effective oscillator frequency $\Omega^2(x_0)$ at the original point of coordinate $x_0 = 0$ is plotted as a function of the inverse temperature. As mentioned, the precision of

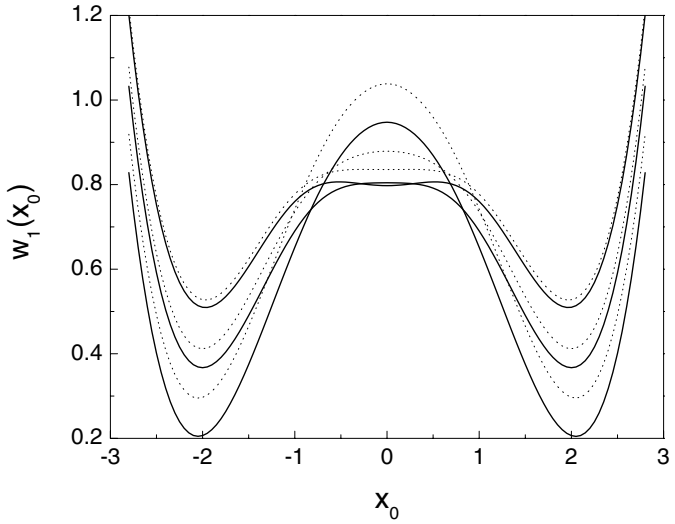

Figure 1. The temperature-dependent ECP. The solid and dotted curves represent our results and those of F–K [4], respectively. The values of β are equal to 5.0, 10.0 and 25.0 from top to bottom.

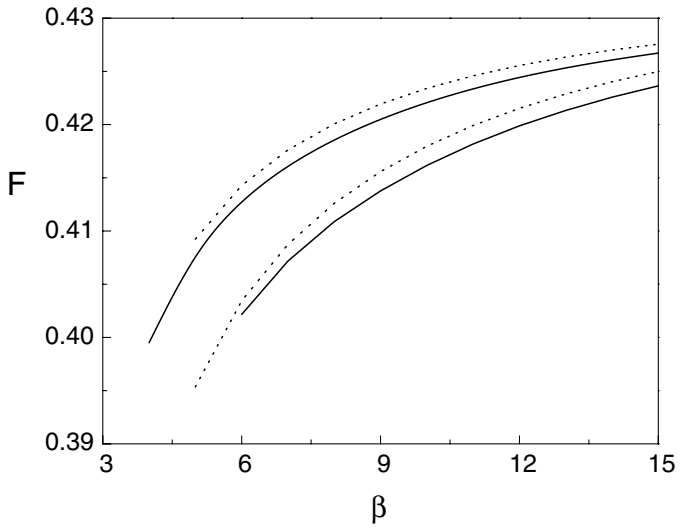

Figure 2. The free energy as a function of the inverse temperature. The solid and dotted curves represent our results and those of F–K [4], respectively. The coupling parameter $g = 0.8$ and 1.2 from top to bottom.

the variational path integral approach can be checked by the oscillator frequency of the ECP. When the temperature approaches zero, the frequency at the bottom of the ECP will become the quantal energy difference of the first excited state and the ground state. In the F–K method, in order to yield convergent results of the path integrals, the oscillator frequency at the saddle point must be larger than the realistic frequency, so the calculated results are always larger than the exact value. For instance, the error is larger than 70% for the double-well potential with a coupling constant $g = 0.4$. It is impossible to obtain the exact expression of the

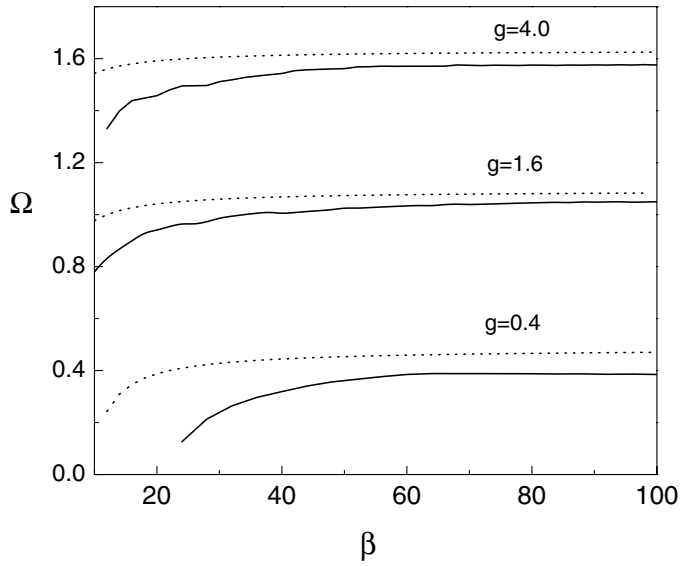

Figure 3. The oscillator frequency of the ECP at $x_0 = 0$ as a function of the inverse temperature for different coupling constants. The solid and dotted curves represent our results and those of F–K [4], respectively.

Table 1. The difference between the first and ground energy levels.

g	ΔE	Ω (our results)	Ω (F–K results)
0.4	0.2969	0.386	0.486
0.8	0.6159	0.701	0.760
1.2	0.8166	0.898	0.948
1.6	0.9730	1.049	1.093
4.0	1.5058	1.575	1.634

oscillator frequency at a low temperature limit, so we must carry out a numerical extrapolation to $T \to 0$. When $g > 0.36$, the barrier of the ECP disappears, and the original double-well potential is changed into a single well. So, we need to calculate the oscillator frequency of the ECP at $x_0 = 0$ only. It is seen from figure 3 that the oscillator frequency of the ECP can approach a constant when the temperature is lowered.

More detailed data are shown in table 1. It is shown that our result is close to the exact value of quantum mechanics [12] compared with the F–K method.

4. Summary

In this paper, we have presented an improvement of the F–K procedure for obtaining an estimate of the minimum energy of a particle in a quantum double-well potential. For a symmetrical double-well potential the ECP was obtained, where the Gaussian expectation is replaced by a non-Gaussian average. In comparison with the previous calculation of the energy-level splitting using the F–K method, the accuracy of the present improved approach is increased by about 50%. It is possible that the expectations of the thermodynamical quantities remain finite when the temperature approaches the crossover temperature, and the higher-order perturbation expansion can be applied safely. Moreover, this procedure is always convergent.

The present approach seems to be quite special and tailored to the double-well problem. It provides an improvement relative to the corresponding F–K procedure and still deviates from the desired results. However, if we consider an equivalent Gaussian distribution, $Z_1^{-1}\exp\left(-m\beta\sum_{n=1}^{\infty} I_n^{-1}X_nX_{-n}\right)$, and combine with a convergent higher-order perturbation expansion, more accurate results may be estimated. Furthermore, we believe that the present method can be employed in the case of tunnelling states. It can also be applied to other potentials, for example, the periodic potential, nonlinear dissipative system, barrier expansion, etc. We should observe more detailed quantum behaviours of a system near the barrier top.

Acknowledgments

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References

[1] Feynman R P and Hibbs A R 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw Hill)
[2] Feynman R P 1972 *Statistical Mechanics* (Reading, MA: Benjamin)
[3] Giachetti R and Tognetti V 1985 *Phys. Rev. Lett.* **55** 912
[4] Feynman R P and Kleinert H 1986 *Phys. Rev.* A **34** 5080
[5] Kleinert H 1990 *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics* (Singapore: World Scientific)
[6] Weiss U 1993 *Quantum Dissipative Systems* (Singapore: World Scientific)
[7] Kleinert H and Meyer H 1994 *Phys. Lett.* A **184** 319
[8] Kleinert H 1994 *Phys. Lett.* A **190** 131
[9] Kleinert H, Kürzinger W and Pelster A 1998 *J. Phys. A: Math. Gen.* **31** 8307
[10] Grabert H, Olschowski P and Weiss U 1987 *Phys. Rev.* B **36** 1931
[11] Calderia A O and Leggett A J 1981 *Phys. Rev. Lett.* **46** 211
[12] Bao J D, Zhuo Y Z and Wu X Z 1995 *Phys. Rev.* E **52** 5656
[13] Bao J D, Abe Y and Zhuo Y Z 1998 *Phys. Rev.* E **58** 2931
[14] Zappalà D 2001 *Phys. Lett.* A **290** 35