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IMPROVING THE GAUSSIAN EFFECTIVE POTENTIAL: QUANTUM MECHANICS[*]

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ABSTRACT

In order to gain intuition for variational problems in field theory, we analyze variationally the quantum–mechanical anharmonic oscillator $\left[V(x) = \frac{k}{2} x^2 + \frac{\lambda}{4} \lambda^4 \right]$. Special attention is paid to improvements to the Gaussian effective potential.

1. INTRODUCTION

The study of spontaneous symmetry breakdown[1] in field theory is usually carried out by the analysis of the effective potential (V_{eff}). In general, V_{eff} can be defined as the minimum expectation value of the system's Hamiltonian $V_{eff}(\phi) = \min_{\{\psi\}} <\psi|H|\psi>$, subjected to the constraints $<\psi|\psi> = 1$ and $<\psi|\Phi|\psi> = \phi$, where Φ is the field operator. The point where V_{eff} is minimum defines the physical theory. As is well known, the effective potential generates the Green's functions at zero momentum and energy.

Since the minimization of $<\psi|H|\psi>$ over the whole functional space is a tremendous task, a very popular field theoretical method for obtaining V_{eff} is the loop expansion[2], which suffers from the shortcoming of being a perturbative expansion. One way to look for some non perturbative effects is to employ the so called "Gaussian effective potential"[3] which is evaluated by minimizing $<\psi|H|\psi>$ over the subspace of Gaussian wave functionals. Gaussian *Ansätze* have also been used to analyze time dependent problems[4] that appear in the description of the early universe.

Although the Gaussian effective potential is very appealing for its simplicity, it is not easy to improve upon since we must enlarge the subspace of the allowed wave functionals and this leads to involved calculations.

In this paper we shall analyze a simple quantum–mechanical system through the effective potential method, in order to gain some intuition that can be applied to field theoretic models. Our goal is to compare the results of the Gaussian approximation with the one obtained by enlarging the class of allowed wave functionals. We shall restrict our attention to trial wave functions that belong to the class of linear combinations of Gaussians or products of Gaussians by polynomials because, with this choice of *Ansätze*,

the computations involved are feasible not only in the quantum mechanical context but also for field theoretic models.

This paper is organized as follows. As a first step, in Sec. II, we obtain the ground state for the quantum–mechanical anharmonic oscillator using several *Ansätze* for the states ψ. Section III contains the analysis of the effective potential obtained for different *Ansätize* Our conclusions are presented in Sec. IV.

2. VARIATIONAL ESTIMATE OF THE GROUND STATE

We shall study the quantum system consisting of a unit–mass anharmonic oscillator subject to a quartic potential, whose Hamiltonian is*:

$$H = \frac{p^2}{2} + V(x) \quad , \tag{2.1a}$$

with p being the momentum operator and

$$V(x) = \frac{k}{2} x^2 + \frac{\lambda}{4} x^4 \quad , \tag{2.1b}$$

where λ is a positive constant, and k may be positive or negative. For $k < 0$ eq.(2.1b) represents the double–well potential, that in Quantum Field Theory is related to spontaneous symmetry breakdown.

The purely Gaussian *Ansatz* has been considered previously as an approximation to the eigenfunction of H associated with the lowest energy[3]. As a warm up for the field theoretical problem, we shall improve the Gaussian *Ansatz* in Quantum Mechanics in order

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*We are using units where: $\hbar = 1$.

to get more precise information on the behaviour of the system described by (2.1).

For fixed $\lambda(=1)$, a qualitative analysis based upon the shape of $V(x)$ suggests the existence of three different intervals of k where the system is expected to exhibit different physical behaviour. For $k > 0$, $V(x)$ has only one minimum and the lowest energy eigenstate is a function with one peak at $x = 0$. Even for small negative values of k ($k \gtrsim -1$) we expect the same one–peak behaviour for the lowest energy eigenstate since its eigenvalue is supposed to be bigger than $V(0)$, so that, the particle is not forced to stay very long in any of the wells.

For moderate negative values of k ($-3 \lesssim k \lesssim -1$), the lowest energy of the system is smaller than $V(0)$, and the only possibility that the particle beginning in one well reachs the other is through tunnelling. In this case, the barrier that the particle has to cross is not thick enough, such that the tunnelling effect is still large. Moreover, the eingenfunction of the lowest state is expected to have two peaks that are not well separated from one another.

For large negative k ($k \lesssim -3$), the barrier that the particle has to cross, when it is initially in one well, in order to get to the other, is very thick and the wave function inside the barrier vanishes so quickly that the system almost behaves as consisting of two independent wells. We need to take this last phrase with caution, because there is always tunnelling in Quantum Mechanics, even though it can be very small.

Now we proceed to make more quantitative the previous considerations. Our first improvement to the Gaussian *Ansatz* is the introduction of a quadratic polynominal multiplying the Gaussian wave function – that is,

$$\psi(x) = \sqrt{N} \left[1 + \beta (x - x_0)^2 \right] e^{-\frac{\omega}{2} (x - x_0)^2} \quad , \tag{2.2}$$

where ω, β and x_0 are variational parameters used to minimize $<\psi | H | \psi>$, and N is

the normalization constant such that ψ has unit norm.

The anharmonic potential given by eq. (2.1b) is obviously invariant under the parity transformation $x \to -x$, so that the ground state is an even function of x. For moderate negative values of k $(-3 \lesssim k \lesssim -1)$, each well of the double–well potential is sufficiently deep to force the ground state eigenfunction to become nodeless endowed with two peaks. For such values of k we can not expect the single–peaked Gaussian *Ansatz* to be a good approximation to the ground state wave function. Therefore we are naturally led to consider the following *Ansatz*:

$$\psi(x) = \sqrt{N} \left\{ \left[1 + \beta(x-x_0)^2 \right] e^{-\frac{\omega}{2}(x-x_0)^2} + B \left[1 + \beta(x+x_0)^2 \right] e^{-\frac{\omega}{2}(x+x_0)^2} \right\}. \quad (2.3)$$

N is a normalization constant such that ψ has norm one, and it is determined in terms of the variational parameters β, x_0, ω and B. The purely Gaussian *Ansatz* is obtained from (2.3) by putting $B = \beta = 0$, and an even wave function is obtained by setting $B=1$. Imposing the normalization condition on ψ, we obtain that

$$N = \frac{\omega^{5/2}}{\sqrt{\pi}} \left\{ (1+B^2) \left[\omega^2 + \beta\omega + \frac{3}{4}\beta^2 \right] + 2B\, e^{-\omega x_0^2} \left[\omega^2 \left[1 + 2\beta x_0^2 + \beta^2 x_0^4 \right] + \right. \right.$$

$$\left. \left. + \frac{\omega}{2} \left[2\beta - 2\beta^2 x_0^2 \right] + \frac{3}{4}\beta^2 \right] \right\}^{-1}. \quad (2.4)$$

Using equations (2.1), (2.3) and (2.4), it is straightforward, but somewhat tedious, to compute

$$E[\psi] = <\psi|H|\psi> , \quad (2.5)$$

which yields

$$E[\psi] = \omega^{-2} \left\{ (1+B^2) \left[\omega^2 + \beta\omega + \frac{3}{4}\beta^2 \right] + 2B\, e^{-\omega x_0^2} \left[\omega^2 \left[1 + 2\beta x_0^2 + \beta^2 x_0^4 \right] + \right. \right.$$

$$\left. + \omega \left[2\beta - \beta^2 x_0^2 \right] + \frac{3}{4}\beta^2 \right] \right\}^{-1} \left\{ (1+B^2) \left[-\frac{1}{4}\beta\omega^4 + \frac{7}{16}\beta^2\omega^3 + \frac{1}{4}\omega^5 + k \left[\frac{1}{4}\omega^3 + \right. \right. \right.$$

$$\left. + \frac{1}{2}\omega^4 x_0^2 + \frac{3}{4}\beta\omega^2 + \frac{1}{2}\beta\omega^3 x_0^2 + \frac{15}{16}\beta^2\omega + \frac{3}{8}\beta^2\omega^2 x_0^2 \right] + \lambda \left[\frac{3}{16}\omega^2 + \frac{3}{4}\omega^3 x_0^2 + \right.$$

$$\left. + \frac{1}{4}\omega^4 x_0^4 + \frac{15}{16}\beta\omega + \frac{9}{4}\beta\omega^2 x_0^2 + \frac{1}{4}\beta\omega^3 x_0^4 + \frac{105}{64}\beta^2 + \frac{45}{16}\beta^2\omega x_0^2 + \frac{3}{16}\beta^2\omega^2 x_0^4 \right] \right] +$$

$$+ B\, e^{-\omega x_0^2} \left[-\frac{1}{2}\beta x_0^4 + \frac{1}{2}\omega^5 + 4\beta\omega^5 x_0^2 - \omega^6 x_0^2 - 2\beta\omega^6 x_0^4 - \frac{25}{4}\beta^2 x_0^2\omega^4 + \right.$$

$$+ \frac{11}{2}\beta^2\omega^5 x_0^4 - \beta^2\omega^6 x_0^6 + \frac{7}{8}\beta^2\omega^3 + k \left[\frac{1}{2}\omega^3 + \beta x_0^2\omega^3 + \frac{1}{2}\beta^2 x_0^4\omega^3 + \frac{3}{2}\beta\omega^2 - \frac{3}{2}\beta^2 x_0^2\omega^2 + \right.$$

$$\left. + \frac{15}{8}\beta^2\omega \right] + \lambda \left[\frac{3}{8}\omega^2 + \frac{3}{4}\beta x_0^2\omega^2 + \frac{3}{8}\beta^2 x_0^4\omega^2 + \frac{15}{8}\beta\omega - \frac{15}{8}\beta^2 x_0^2\omega + \frac{105}{32}\beta^2 \right] \right] \right\} . \quad (2.6)$$

For fixed values of k and λ we can get an approximation to the ground state energy E_0 by finding the values of the parameters β, ω, x_0 [for $B = 0, 1$] for which $E[\psi]$ is minimized. This is achieved by requiring that the partial derivate of $E[\psi]$ with respect to each of these parameters to be zero. However, in this fashion we obtain coupled nonlinear algebraic equations that are too intrincate to be solved analytically. Therefore, for fixed k and λ we determine numerically the set of parameters that minimize (2.6).

So long as only the relative values of k and λ are important, we shall set $\lambda = 1$ from now on (with the consequence that the location $\left(\pm \sqrt{-\frac{k}{\lambda}} \right)$ and depth $\left(-\frac{k^2}{4\lambda} \right)$ of the minima of $V(x)$ are determined by k alone).

We compare the numerical results for the minimum value of $E[\psi]$ for the following

Ansätze: Gaussian ($\beta = 0$, B $= 0$), sum of two Gaussians ($\beta = 0$, B $= 1$), one quadratic correction (B $= 0$) and a symmetric quadratic correction (cf. eq.(2.3) with B $= 1$). The numerical analysis is made for two values of k that give rise to a single–well potential (k $= 0$ and 1) and for six values of k for which the potential (2.1b) possesses two wells. The latter situation is expected to exhibit a more interesting behaviour. In Table 1 we display the approximate values of the ground state energy for each of the four previous *Ansätze*. Table 2 contains the relative corrections afforded by the other three trial functions with respect to the Gaussian *Ansatz* (B $= 0$ and $\beta = 0$).

From the numerical results, we learn that, in the interval k $\gtrsim -1$, where the eigenfunction has an one–peaked form (see for example Figure 1), the best wave function of the three *Ansätze* (2.2), (2.3) with B $= 0$ and B $= 1$, are flatter and broader than the Gaussian *Ansatz* in the region around x $= 0$. Moreover, they vanish faster than the Gaussian *Ansatz* for large x , and the *Ansätze* considered yield almost the same value for the ground state energy. We should remember that for this interval of k the approximate lowest energies are positive and there is no classically forbidden region.

In Figure 2 we present an example of best fit wave function for k $= -2.0$, that illustrates a typical behaviour for $-3 \lesssim$ k $\lesssim -1$. For this interval of k the three *Ansätze* have a two–peaked form while the Gaussian one has only one maximum. Therefore, there is a qualitative difference between the three new *Ansätze* and the Gaussian *Ansatz*, in this interval of k : from the shape of the trial wave functions, we see that the quantum tunnelling effect is very important and each well "feels" the presence of the other. The best fit of the sum of two Gaussians is very close to the best one using a quadratic correction to a Gaussian, while the symmetric quadratic correction wave function is flatter in the region around the two maxima of the wave function than the *Ansätze* (2.2) and (2.3) with $\beta = 0$ and B $= 1$. Between the two extrema of the wave functions, the symmetric quadratic correction wave function is slightly bigger than the others, and it contains more information about the tunnelling phenomenon.

Finally we shall discuss typical best fit of the four *Ansätze* for k $\lesssim -3$. In this interval of k , the best fit of the Gaussian *Ansatz* and the quadratic correction one are very close, and both exhibit only one peak. These wave functions constrain the particle to stay in only one well, but this is not a correct picture, since there is always tunnelling, besides the fact that the ground state wave function must be symmetric under the change x $\to -$ x . The *Ansätze* (2.3) with B $= 1$ and $\beta = 0$ (sum of two Gaussians) and (2.3) with B $= 1$ (the symmetric quadratic correction) are virtually undistinguishable. It should be noticed that the tunnelling effect is very small, even though it is not exactly zero, and the ground state wave function can be regarded as a nearly incoherent sum of two wave functions localized in disconnected wells. From Table 1 we verify that the minima of $<\psi|H|\psi>$ furnished by each of the four *Ansätze* are very close to each other and this happens because a single Gaussian centered at one of the minima gives the same result as the sum of two independent Gaussians, each centered at one of the minima. For normalization reasons, the maximum value of the single Gaussian is higher by the factor $\sqrt{2}$ than the maximum value of the double Gaussian, and this is clearly shown in Figure 3.

For k $\lesssim -4$, we conclude that the quadratic correction is not a significantly improved *Ansatz* for the ground state neither the symmetric quadratic correction is an improvement to the sum of two Gaussians.

3. APPROXIMATE EFFECTIVE POTENTIAL FROM DIFFERENT *ANSÄTZE*

The effective potential V_{eff} for quantum mechanical systems is defined as[1,5]

$$V_{eff}(<x>) = \min_{\{\psi\}} <\psi|H|\psi> , \qquad (3.1a)$$

where the minimization is performed over all states $|\psi>$ such that,

$$<\psi|x|\psi> = <x> \quad , \tag{3.1b}$$

where $<x>$ is fixed, and the states are properly normalized — that is,

$$<\psi|\psi> = 1 \quad . \tag{3.1c}$$

The potential $V(x)$ that we are considering (see expression (2.1b)) is symmetric under the transformation $x \to -x$, but the expectation value of x is fixed, hence the wave function that minimizes (3.1a) does not have definite parity.

We have computed the approximate effective potential in three cases: the Gaussian effective potential[3] where the space of functions is given by (2.2) with $\beta = 0$; the quadratic correction to the Gaussian *Ansatz*, whose space of functions is given by (2.2), x_0 being the expectation value of x; and finally, the last *Ansatz* is the sum of two Gaussians (expression (2.3) with $\beta = 0$).

Let us begin by the approximate effective potential derived from the normalized quadratic correction to the Gaussian *Ansatz*,

$$\psi(x) = \left[\frac{\omega^{5/2}}{\pi^{1/2}(\omega^2 + \beta\omega + \frac{3}{4}\beta^2)} \right]^{1/2} \cdot \left[1 + \beta(x-x_0)^2 \right] e^{-\frac{\omega}{2}(x-x_0)^2} \quad , \tag{3.2}$$

where ω and β are the variational parameters and x_0 is equal to $<\psi|x|\psi>$, which is fixed. This approximation to the effective potential $V_{eff}(x_0)$ is obtained by means of

$$V_{eff}(x_0) = \min_{\{\omega,\beta\}} <\psi|H|\psi> \tag{3.3a}$$

where*

$$<\psi|H|\psi> = \omega^{-2} \left[\omega^2 + \beta\omega + \frac{3}{4}\beta^2 \right]^{-1} \cdot \left\{ -\frac{1}{4}\beta\omega^4 + \frac{7}{16}\beta^2\omega^3 + \frac{1}{4}\omega^5 + \right.$$

$$+ k\left[\frac{1}{4}\omega^3 + \frac{1}{2}\omega^4x_0^2 + \frac{3}{4}\beta\omega^2 + \frac{1}{2}\beta\omega^3x_0^2 + \frac{15}{16}\beta^2\omega + \frac{3}{8}\beta^2\omega^2x_0^2 \right] +$$

$$+ \lambda\left[\frac{3}{16}\omega^2 + \frac{3}{4}\omega^3x_0^2 + \frac{1}{4}\omega^4x_0^4 + \frac{15}{16}\beta\omega + \frac{9}{4}\beta\omega^2x_0^2 + \frac{1}{4}\beta\omega^3x_0^4 + \right.$$

$$\left.\left. + \frac{105}{64}\beta^2 + \frac{45}{16}\beta^2\omega x_0^2 + \frac{3}{16}\beta^2\omega^2x_0^2 \right] \right\} \quad . \tag{3.3b}$$

The Gaussian effective potential is found by setting $\beta = 0$ in (3.3), since in this case we recover the normalized Gaussian *Ansatz* in (3.2).

The third *Ansatz* that we consider is the sum of two Gaussians,

$$\psi(x) = \sqrt{N} \left\{ e^{-\frac{\omega_1}{2}(x-x_1)^2} + B\, e^{-\frac{\omega_2}{2}(x-x_2)^2} \right\} \quad , \tag{3.4a}$$

where $\omega_1, \omega_2, x_1, x_2$ and B are variational parameters. We should remember that for $<x>$ fixed the lowest energy eigenstate is not necessarily an even function of x. The normalization constant N, such that $<\psi|\psi> = 1$, is given by

$$N = \frac{1}{\sqrt{\pi}} \left\{ \frac{1}{\sqrt{\omega_1}} + \frac{B^2}{\sqrt{\omega_2}} + \frac{\sqrt{8}\,B}{\sqrt{\omega_1+\omega_2}} e^{-\frac{\omega_1\omega_2}{2(\omega_1+\omega_2)}(x_1-x_2)^2} \right\}^{-1} \quad . \tag{3.4b}$$

---

*For the sake of completeness, we are exhibiting all the following expressions for arbitrary λ, although we use $\lambda=1$ in the numerical work.

The expectation value of H for the space of trial functions (3.4) is

$$
<\psi|H|\psi> = \frac{N\sqrt{\pi}}{2}\left\{\frac{\sqrt{\omega_1}}{2} + k\left[\frac{1}{2\omega_1^{3/2}} + \frac{x_1^2}{\omega_1^{1/2}}\right] + \frac{\lambda}{2}\left[\frac{3}{4\omega_1^{5/2}} + \frac{3x_1^2}{\omega_1^{3/2}} + \frac{x_1^4}{\omega_1^{1/2}}\right] + \right.
$$

$$
+ B^2\left[\frac{\sqrt{\omega_2}}{2} + k\left[\frac{1}{2\omega_2^{3/2}} + \frac{x_2^2}{\omega_2^{1/2}}\right] + \frac{\lambda}{2}\left[\frac{3}{4\omega_2^{5/2}} + \frac{3x_2^2}{\omega_2^{3/2}} + \frac{x_2^4}{\omega_2^{1/2}}\right]\right] +
$$

$$
+ 2B\sqrt{\frac{2}{\omega_1+\omega_2}}\, e^{-\frac{1}{2}\frac{\omega_1\,\omega_2}{\omega_1+\omega_2}(x_1-x_2)^2}\left[\frac{\omega_1\,\omega_2}{\omega_1+\omega_2} + \omega_1\omega_2\,\bar{y}^2 - \omega_1\omega_2(x_1+x_2)\bar{y} + \right.
$$

$$
\left.\left. + x_1x_2\,\omega_1\omega_2 + k\left[\frac{1}{\omega_1+\omega_2} + \bar{y}^2\right] + \frac{\lambda}{2}\left[\frac{3}{(\omega_1+\omega_2)^2} + \frac{6\bar{y}^2}{\omega_1+\omega_2} + \bar{y}^4\right]\right]\right\}, \quad (3.5a)
$$

where N is given by (3.4b) and

$$
\bar{y} = \frac{x_1\omega_1 + x_2\omega_2}{\omega_1 + \omega_2}. \tag{3.5b}
$$

The parameter B can be written as a function of the expectation value $<x>$, and the other variational parameters,

$$
B = \left[\frac{\sqrt{\omega_2}}{x_2 - <x>}\right]\cdot\left\{-\sqrt{\frac{2}{\omega_1+\omega_2}}\, e^{-\frac{\omega_1\,\omega_2}{2(\omega_1+\omega_2)}(x_1-x_2)^2}\cdot(\bar{y}-<x>) \pm\right.
$$

$$
\pm\left[\frac{2(\bar{y}-<x>)^2}{\omega_1+\omega_2}\, e^{-\frac{\omega_1\,\omega_2}{(\omega_1+\omega_2)}(x_1-x_2)^2} - \frac{(x_2-<x>)(x_1-<x>)}{\sqrt{\omega_1\omega_2}}\right]^{1/2}\right\}, \tag{3.6}
$$

where the sign of the square root that appears in (3.6) is chosen such that (3.5) gives the minimum for $<x>$ fixed.

Again we have three distinct behaviours of the approximate effective potential depending on the value of k. For $k \gtrsim -1.5$ the three approximate effective potentials are convex and they are equal for $x \gtrsim x_{cl}$, where x_{cl} ($\sqrt{-\frac{k}{\lambda}}$) is the classical minimum of V(x), and the quantum corrections are negligible. For a typical behaviour of these approximations, see Figure 4 where we have $k = -1$. We notice that the approximate effective potential yielded by the trial wave function (3.2) is lower than the Gaussian effective potential, as it should be, since it contains more variational parameters.

For $-3 \lesssim k \lesssim -1.5$ we show some typical behaviour in Figure 5 for $k = -2$. Notice that in the classical region $(x_{cl} \gtrsim \sqrt{2})$ the three Ansätze give the same result, but in the region $0 \leq x \lesssim x_{cl}$, the Gaussian effective potential and the one quadratic correction effective potential are no longer convex, whereas the sum of two Gaussians still gives a convex potential.

For the last region of k (i.e., $k \lesssim -3$) we exhibit the typical behaviour in Figure 6 where we have chosen $k = -4$. In the classical region the three Ansätze give the same result, however for $0 \leq x \lesssim x_{cl}$ the Gaussian effective potential is non-convex and the approximate effective potentials obtained using the sum of two Gaussians or the quadratic polynomial times a Gaussian are virtually identical. The effective potential coming from the sum of two Gaussians, or in the same way, the one coming from the one quadratic correction, are nearly convex, see Figure 6. This can be understood from the fact that, in the absence of tunnelling, as happens in field theory, the sum of two Gaussians corresponds to a Maxwell construction for the effective potential[6]. However, this is not the correct realization of the system, since in Quantum Mechanics there is no symmetry breakdown[7]. It must be stressed that we are in the interval of k such that the barrier between the two classical minima is very thick, and the two Ansätze (3.2) and (3.4) are not good enough to

take into account the tunnelling effect that is always present Quantum Mechanics. Therefore for $k \lesssim -3$ none of the three *Ansätze* leads to a reasonable description when we have a double well potential.

4. DISCUSSION

The Gaussian *Ansatz* was applied to Quantum Mechanics and it is quite easily extended to Quantum Field Theory in the Schrödinger Picture[8]. However, if one is interested in improving this *Ansatz*, perhaps the simplest extension amounts to taking the product of a quadratic polynomial by the Gaussian function. The presence of the quadratic term makes the calculations more involved, and the aim of this work is to compare the *Ansatz* (2.3) with the Gaussian one and also with another trial function in the form of a symmetric sum of two Gaussians.

From Tables 1 and 2 we can infer the range of k in which it is important to consider (2.3), and where it can be replaced quite effectively by the symmetric sum of Gaussians:

For positive k, it is clear that the Gaussian *Ansatz* is pretty good. In these cases the quadratic correction to the Gaussian *Ansatz* makes the wave function flatter around its maximum and a little broader than the Gaussian. Moreover, the wave function goes quickly down to zero. The inclusion of an x^2 term to correct the Gaussian *Ansatz* is unimportant because it is dominated by the rapid decrease of the exponencial function.

For small negative k ($k \gtrsim -1$) the ground state energy is positive and there is no tunnelling. The wave function still has one-peaked form whose maximum is at $x = 0$. However, for $-3 \lesssim k \lesssim -1$ the tunnelling effect becomes important. A rough estimate of the probability of tunnelling P can be obtained by using the WKB method[9]. For instance, for $k = -1.5, -2, -3.2$, and -4 we have that $P \simeq 0.5, 0.2, 3 \times 10^{-3}$, and 10^{-4},

respectively. In the region $-3 \lesssim k \lesssim -1$ the Gaussian *Ansatz* is not good at all and the *Ansatz* (2.3) provides a better approximation.

For large negative k ($k \lesssim -3$) the sum of two Gaussians wave function coincides with the one obtained from the family of trial functions (2.3). So long as the computations including the quadratic correction to the Gaussian *Ansatz* are more complicated but lead to no significant improvement of the ground state energy, in this region of k values, thus it is completely unjustified to start with eq. (2.3) with $\beta \neq 0$. In the case $k = -4$, for instance, the ground state energy is effectively the same whether one starts from the trial function (2.3) or simply from a linear combination of two Gaussians, that is, eq. (2.3) with $\beta = 0$.

The approximate effective potentials that are derived with the three *Ansätze* (3.2) (with $\beta = 0$ and $\beta \neq 0$) and (3.4) behave differently for distinct regions of k. For $k \gtrsim -1$ there is no tunnelling effect and the three *Ansätze* give convex effective potential curves. They are all equal in the classically allowed region, $|x| \gtrsim x_{cl}$ where x_{cl} is the positive classical minimum of $V(x)$ and the effective potential derived from the quadratic correction is lower than the one obtained using the Gaussian *Ansatz*, as it should be.

For $-3 \lesssim k \lesssim -1$, the tunnelling effect is very important, and the quadratic correction takes into account this phenomenon. Both the Gaussian effective potential and the quadratic correction one become non-convex while the effective potential coming from the two-Gaussian *Ansatz* is convex. Please notice from Figure 5 that the two-Gaussian effective potential is always lower than the Gaussian and the quadratic correction ones. Furthermore, for small x the two-Gaussian effective potential is almost identical to the quadratic correction one.

For $k \lesssim -3$, the quadratic correction and the sum of two Gaussians give a picture where there is spontaneous symmetry breakdown in Quantum Mechanics, since the effective potential that we obtain in these *Ansätze* is a Maxwell construction, as we have in the broken $\lambda\phi^4$ in Quantum Field Theory. Since there is no spontaneous symmetry

breaking in Quantum Mechanics, these *Ansätze* are not completely satisfactory for $k \lesssim -3$. The reason for this unphysical behaviour is that tunnelling is very small for this range of k since the barrier between the classically allowed regions is thick. However, the quadratic Gaussian and the two—Gaussian effective potentials give arise to a better physical picture than the Gaussian one since they yield no false vacuum and their value at $x = 0$ is much smaller than the one for the Gaussian approximation.

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FIGURE CAPTIONS

Figure 1: Comparison of the different *Ansätze* (solid lines) with the Gaussian one (dot–dashed line) for $\lambda = 1$ and $k = -1$: a) sum of two Gaussians; b) quadratic correction to a Gaussian; c) *Ansatz* (2.3).

Figure 2: Comparison between different *Ansätze* for $k = -2$ and $\lambda = 1$: a) Gaussian (solid line) and sum of two Gaussians (dot–dashed line); b) Gaussian (solid line) and quadratic correction to a Gaussian (dot–dashed line); c) Gaussian (solid line) and the *Ansatz* (2.3) (dot–dashed line); d) sum of two Gaussians (solid line) and the *Ansatz* (2.3) (dot–dashed line).

Figure 3: Same as Fig. 2 for $k = -4$ and $\lambda = 1$: a) Gaussian (solid line) and quadratic correction to a Gaussian (dot–dashed line); b) Gaussian (solid line) and the *Ansatz* (2.3) (dot–dashed line); c) Gaussian (solid line) and the sum of two Gaussians (dot–dashed line); d) sum of two Gaussians (solid line) and the *Ansatz* (2.3) (dot–dashed line).

Figure 4. Effective potential obtained with the *Ansatz* (3.4) for $\lambda = 1$ and $k = -1$.

Figure 5. Effective potential obtained using several *Ansätze* for $\lambda = 1$ and $k = -2$: Gaussian (dashed line), polynomial times a Gaussian (dotted line), and *Ansatz* (3.4) (solid line).

Figure 6. Same as in Fig. 5 but for $\lambda = 1$ and $k = -4$.

Table 1

E_0

k	B=0, β=0	B=1, β=0	B = 0	B = 1
1.0	0.62402	0.62105	0.62106	0.62093
0.0	0.42927	0.42119	0.42124	0.42083
−0.1	0.40716	0.39809	0.39814	0.39775
−1.0	0.17782	0.14800	0.14932	0.14743
−1.5	0.02062	−0.03882	−0.03778	−0.04236
−2.0	−0.16376	−0.28911	−0.28522	−0.29869
−3.2	−1.36046	−1.38061	−1.36051	−1.38062
−4.0	−2.63270	−2.63742	−2.63551	−2.63660

E_0 is the minimum value of $<\psi|\,H\,|\,\psi>$ for the four *Ansätze* and $\lambda = 1$. The Gaussian *Ansatz* is $B = 0$ and $\beta = 0$; the sum of two Gaussians is $B = 1$ and $\beta = 0$; the one quadratic correction is $B = 0$, and finally, the symmetric quadratic correction is $B = 1$.

Table 2

$$\Delta E\%$$

k	B=1, β=0	B = 0	B = 1
1.0	0.47%	0.50%	1.97%
0.0	1.90%	1.90%	1.97%
−0.1	2.20%	2.20%	2.30%
−1.0	16.20%	16.03%	17.09%
−1.5	288%	283%	307.80%
−2.0	76.54%	74.17%	82.39%
−3.2	1.48%	0.34%	1.48%
−4.0	0.20%	0.10%	0.15%

This table shows the relative difference of lowest energy for the three *Ansätze*: sum of two Gaussians, the one quadratic correction and the symmetric quadratic correction, to the Gaussian *Ansatz*, where:

$$\Delta E\% = 100 \; \frac{E_0(B=0, \beta=0) - E_0}{E_0(B=0, \beta=0)} \quad .$$
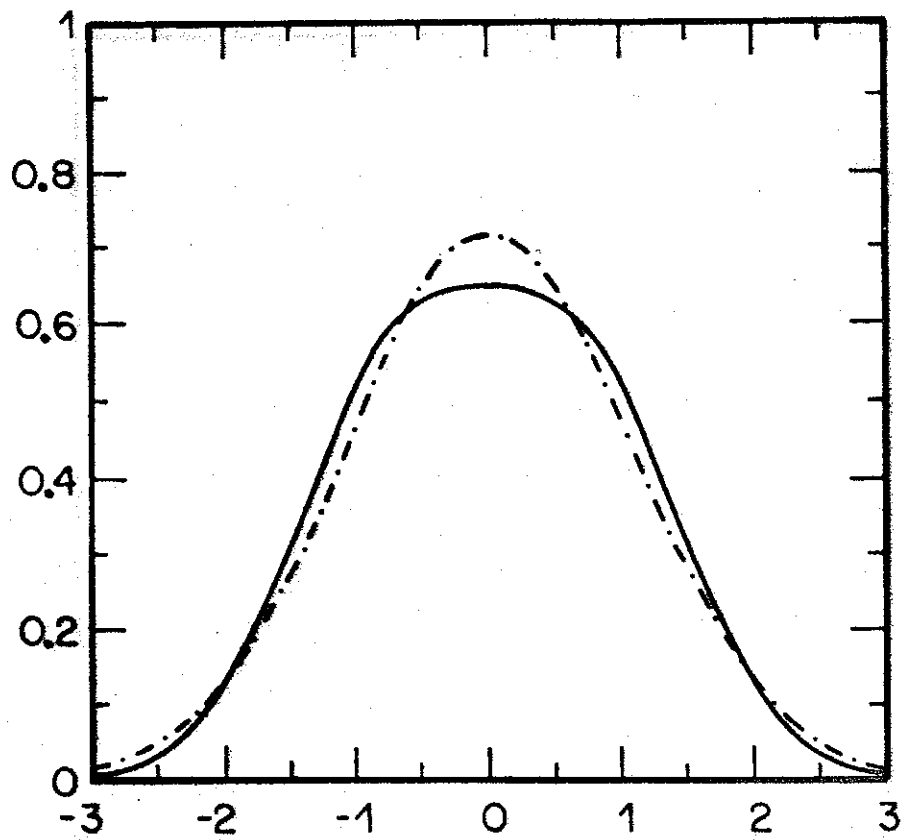
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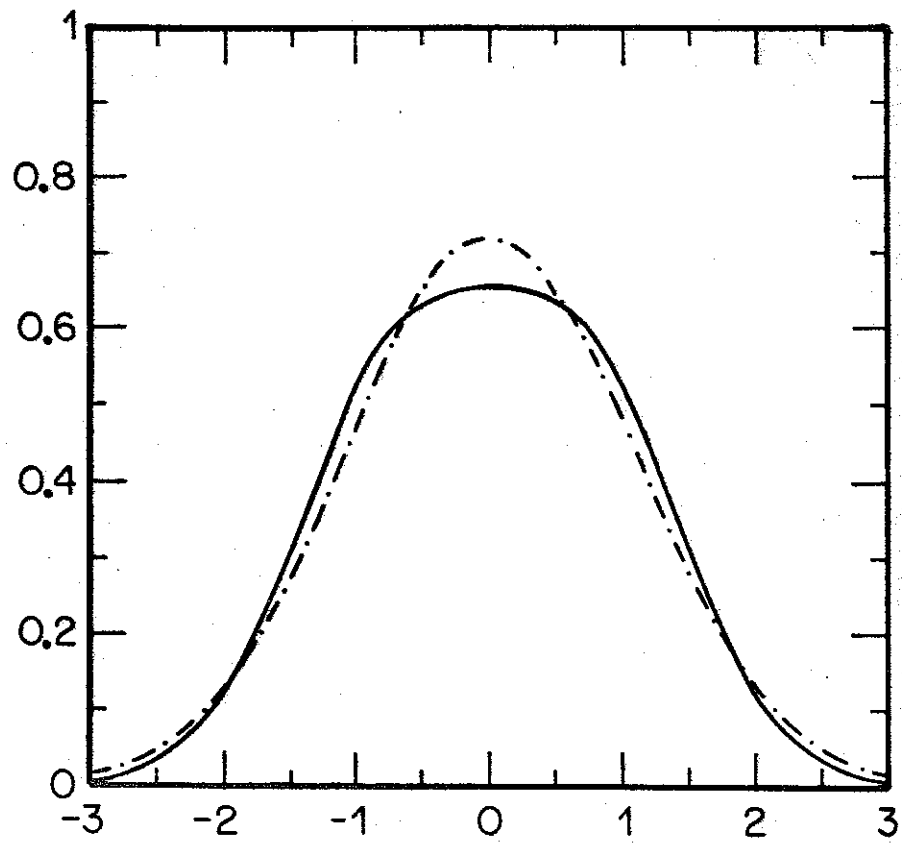
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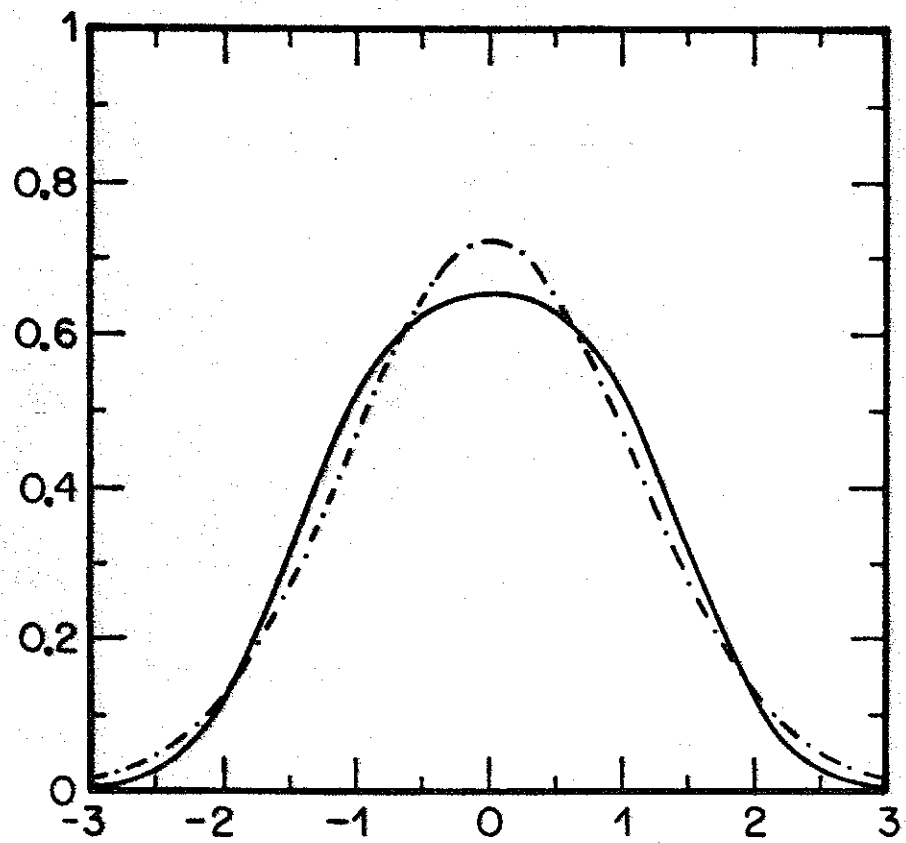
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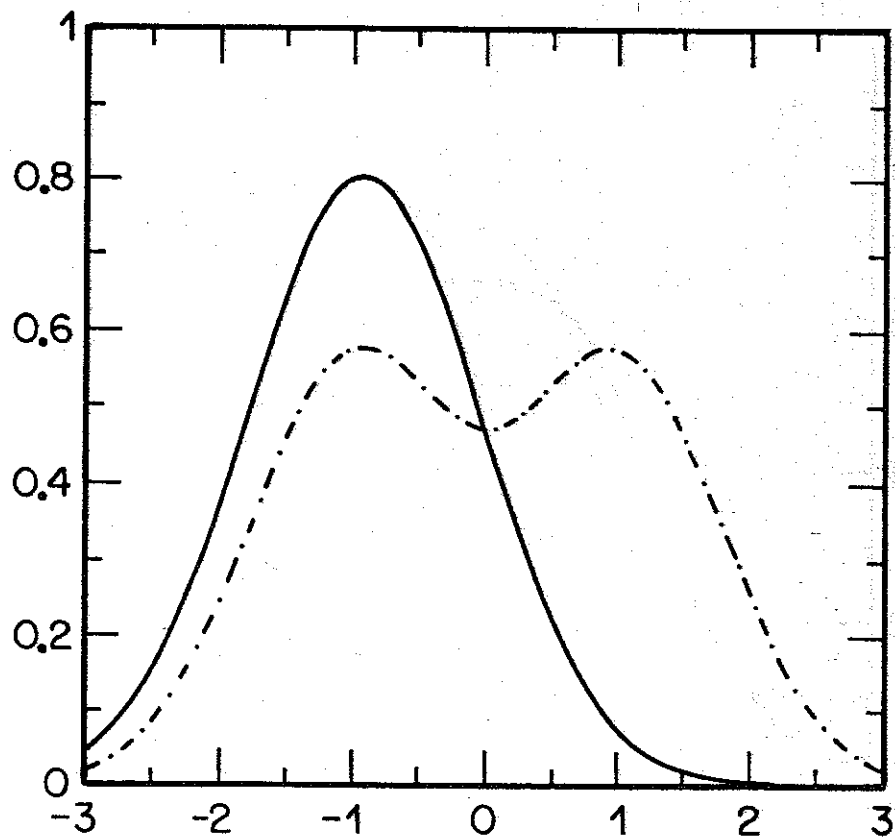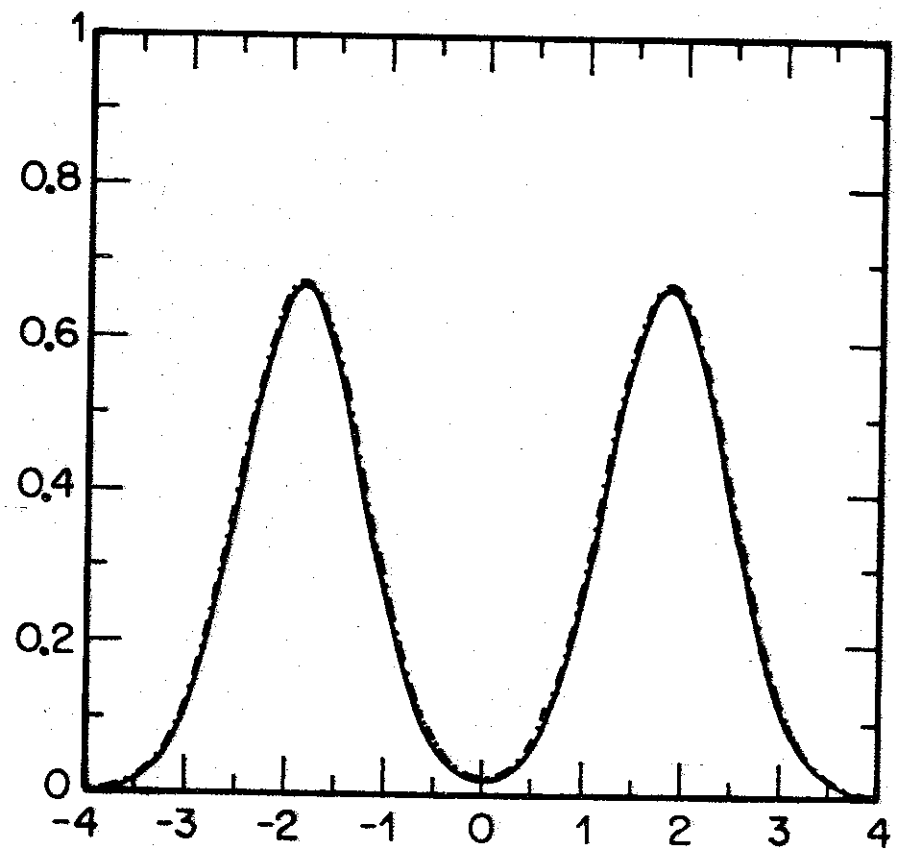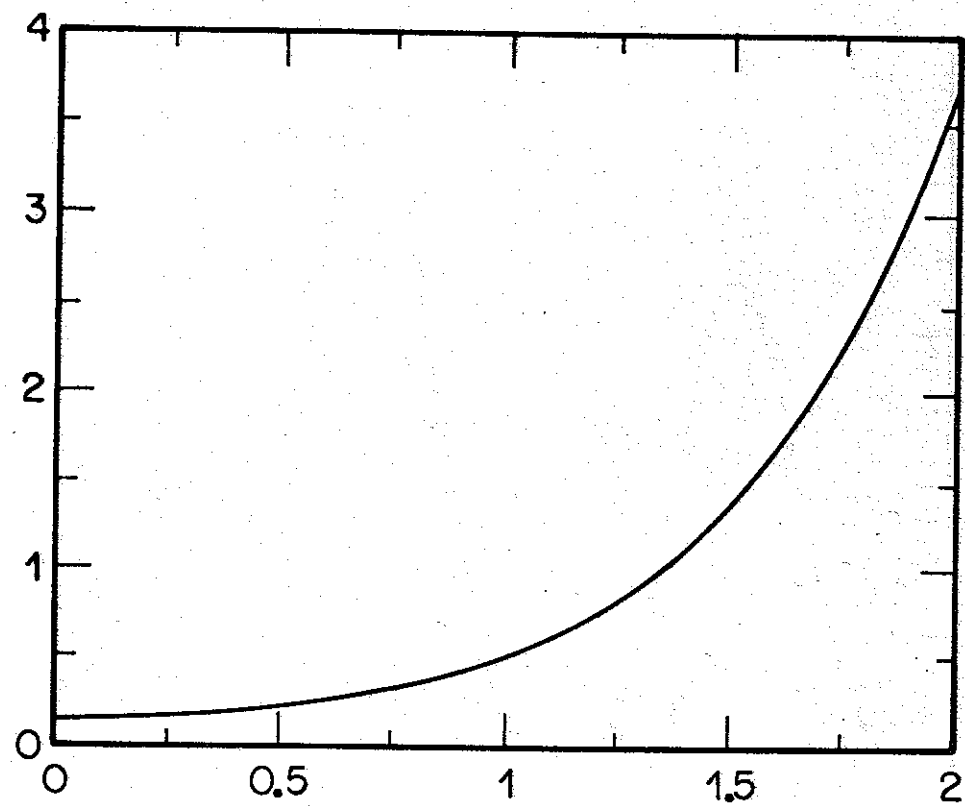
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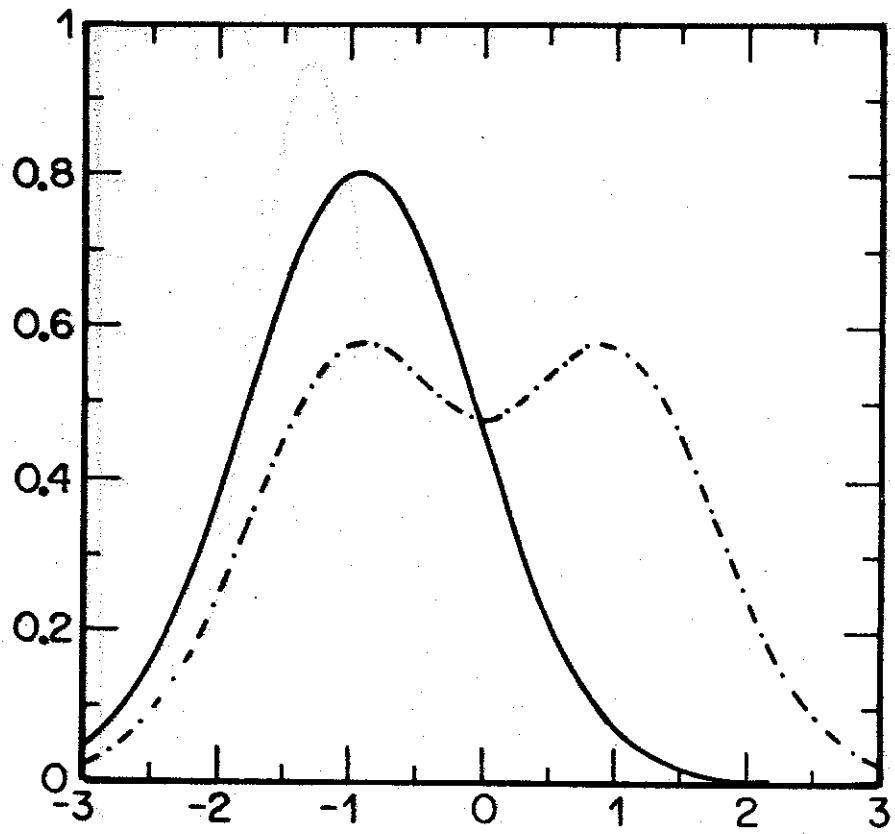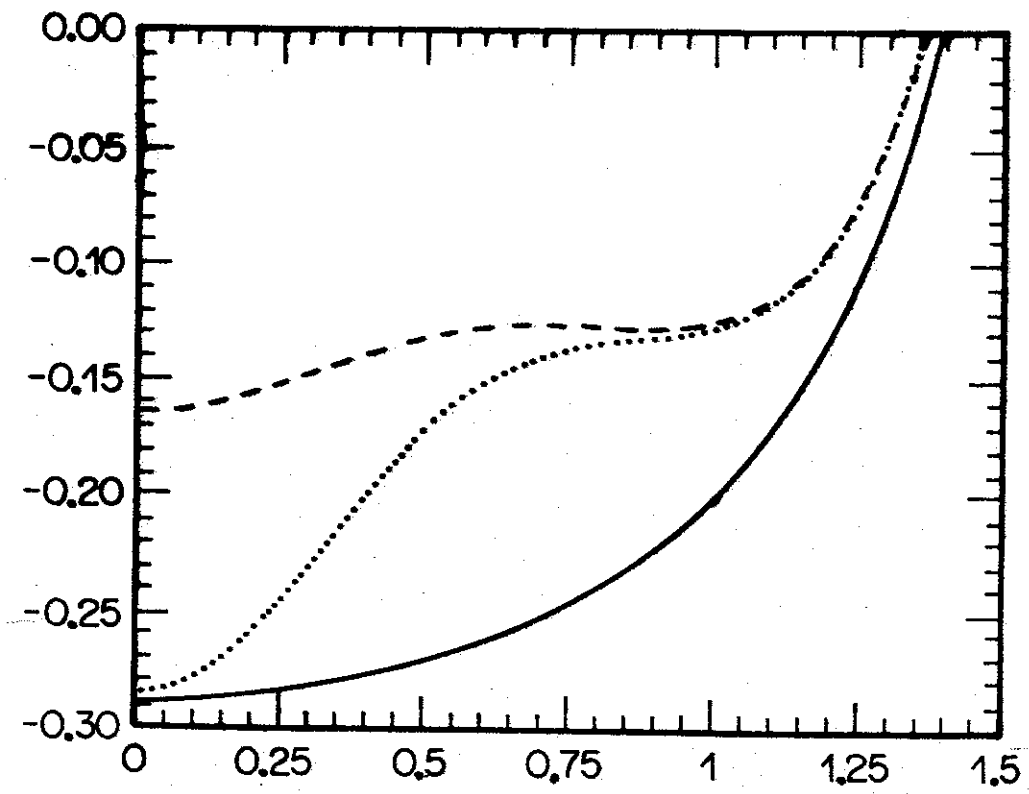
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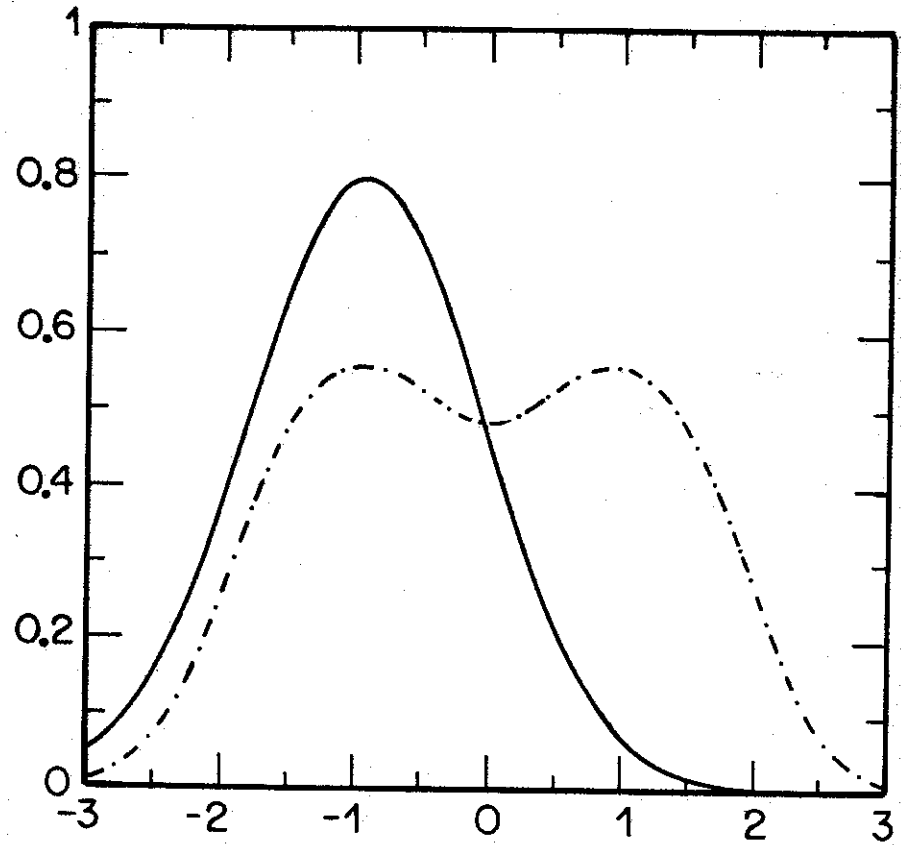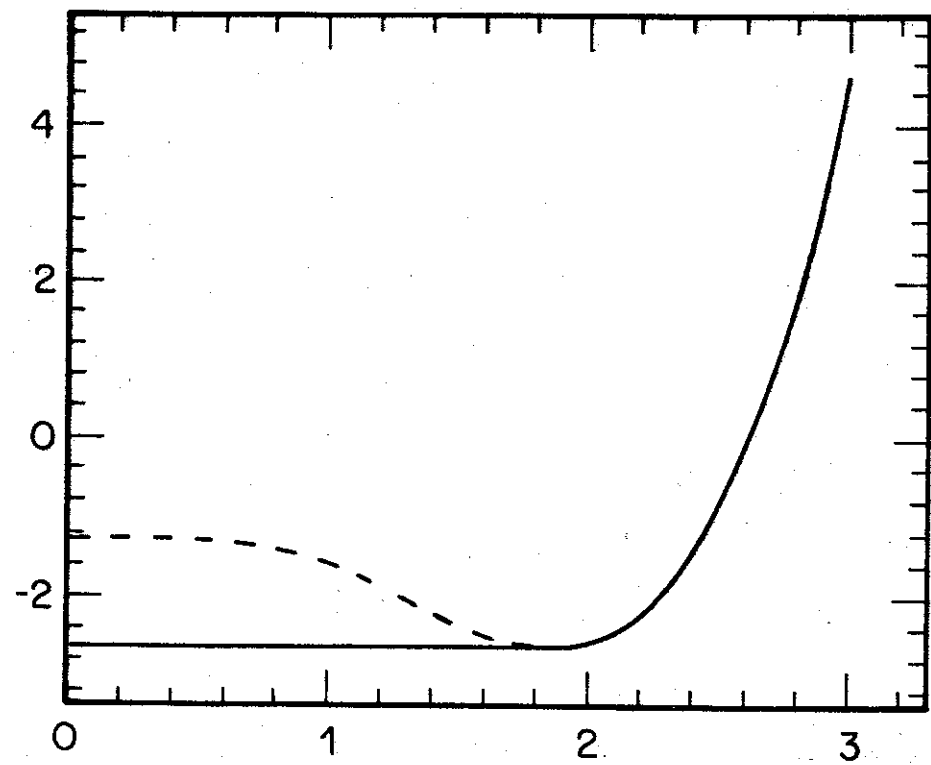
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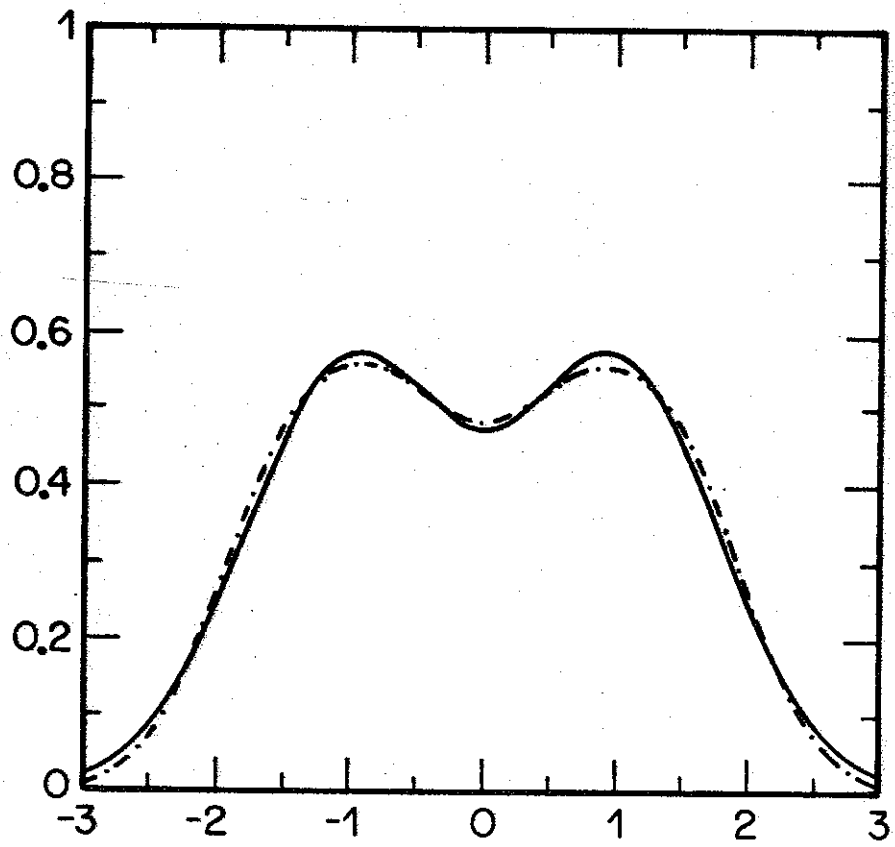
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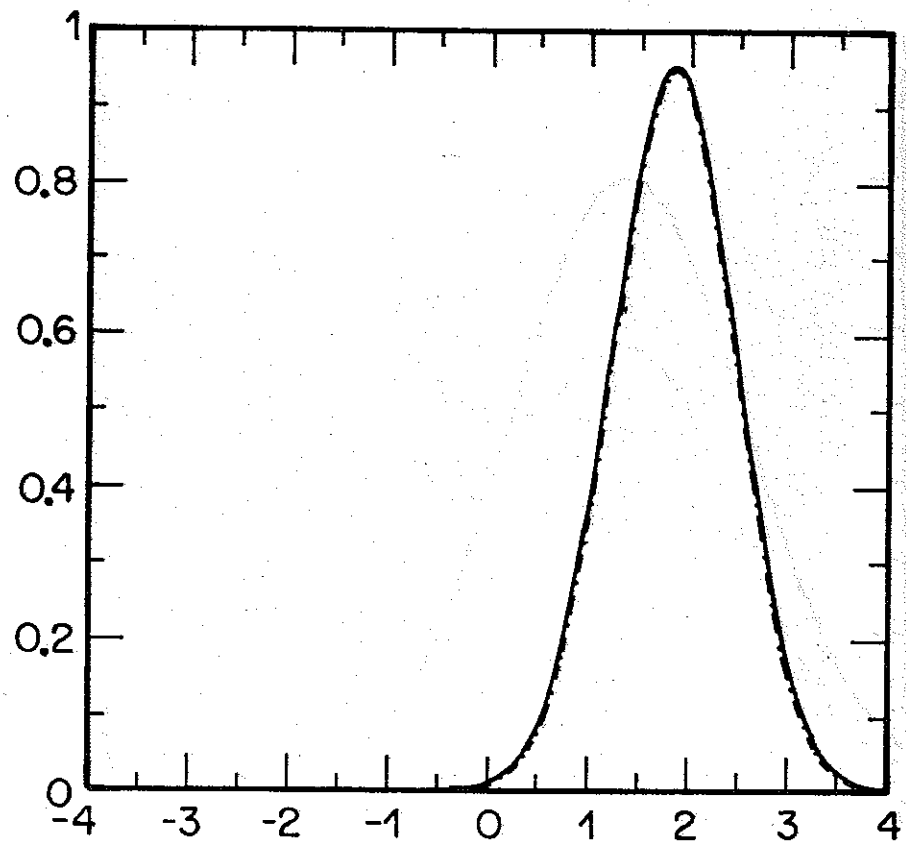
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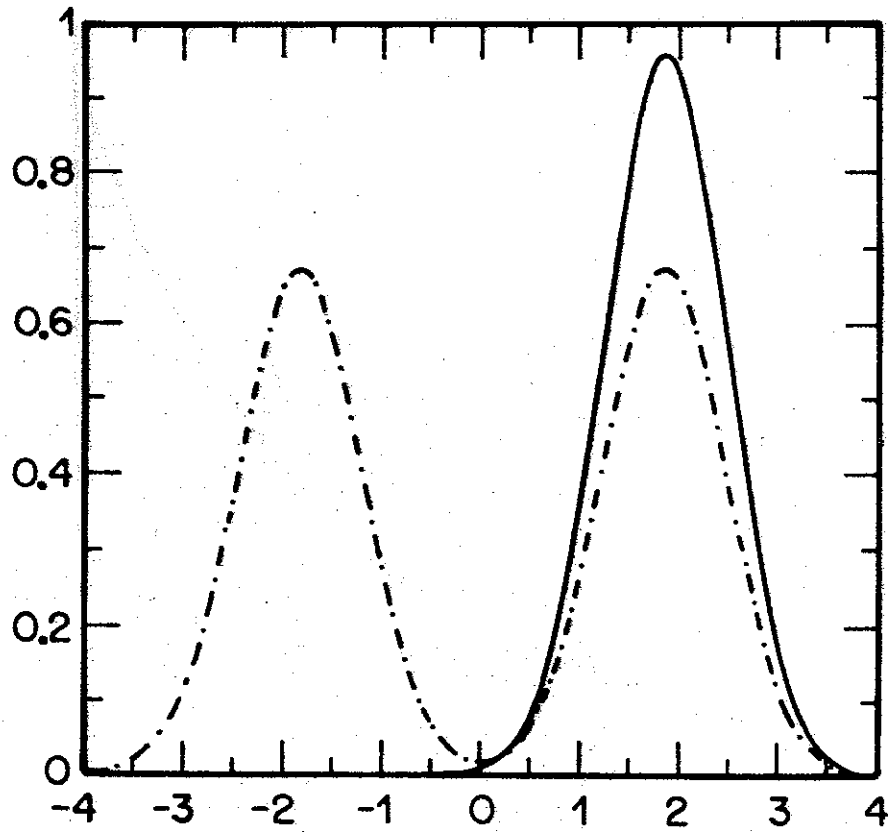
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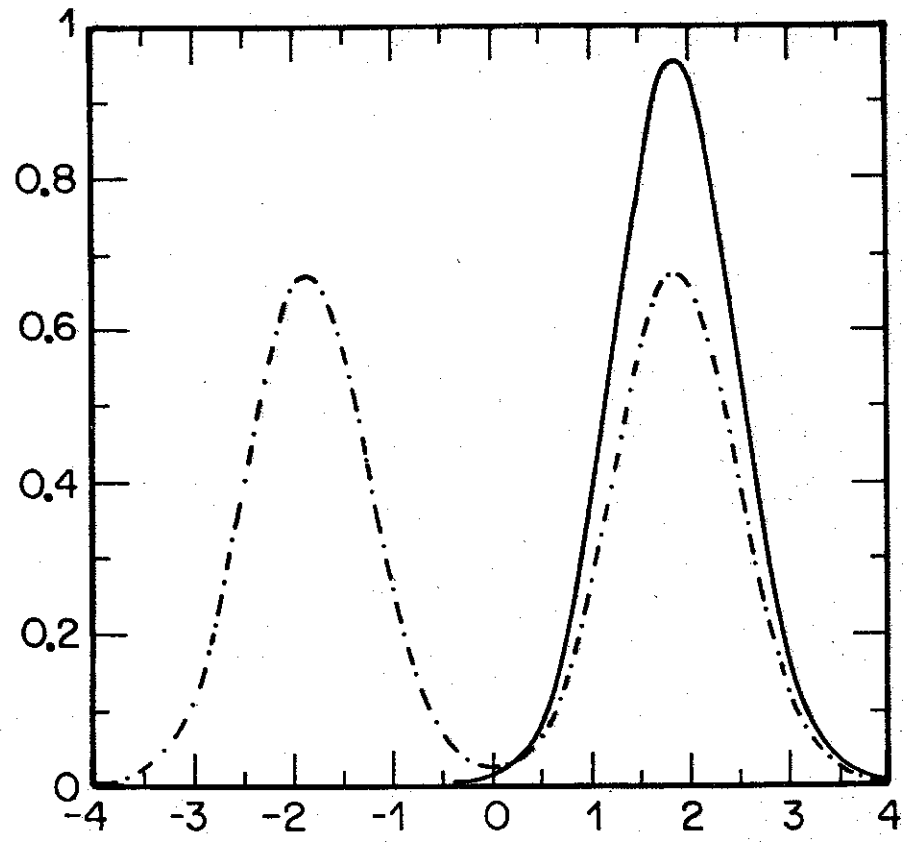
Figure 3.c

Figure 3.d

Figure 4

Figure 5

Figure 6