Feynman-Kleinert's Treatment of a Class of Harmonic-Oscillators

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Z. Naturforsch. **47a**, 1013–1016 (1992); received June 26, 1992

The Feynman-Kleinert method is applied to the harmonic oscillator class of potentials obtained through the factorization method. It is found that the free energy is in good agreement with the exact energy of the harmonic oscillator

The purpose of this paper is to apply the Feynman-Kleinert method [1, 2] to a class of potentials related to the harmonic oscillator and obtained through the so-called factorization method [3]. The exact analytic calculation of the propagator via path integral approach is not quite up to scratch yet, despite considerable progress in this field thanks to the introduction of the time parameter [4] and to the reparametrization of paths.

Let us keep in mind that the very principle of the Feynman-Kleinert method consists in using the path-integral representation of the partition function [5] in quantum mechanics, namely in standard notations,

$$\begin{aligned} Z &= \exp(-\beta F) \\ &= \int \mathscr{D}\, x(\tau) \exp\left\{-\int_0^\beta \mathrm{d}\tau \left(\frac{\dot{x}^2(\tau)}{2} + V(x(\tau))\right)\right\} \\ &= \int \frac{\mathrm{d}x_0}{(2\pi\beta)^{1/2}} \left[\prod_{n=1}^{\infty} \int \frac{\mathrm{d}x_n^{\mathrm{real}}\,\mathrm{d}x_n^{\mathrm{im}}}{\pi/(\beta\omega_n^2)} \right. \qquad (1) \\ &\qquad \left. \cdot \exp\left\{-\beta \sum_{n=1}^{\infty} \omega_n^2 |x_n|^2 - \int_0^\beta \mathrm{d}\tau\, V(X(\tau))\right\}\right], \end{aligned}$$

with $\omega_n = 2\pi n/\beta$.

Integrations over x_n^{real} and x_n^{im}, for $n>0$, converge fast, leaving only the integration over x_0,

$$Z = \int \frac{\mathrm{d}x_0}{(2\pi\beta)^{1/2}} \exp\{-\beta\, w(x_0)\}\,, \qquad (2)$$

where

$$w(x_0) \approx w_1(x_0) = \min[\tilde{w}_1(x_0, a^2(x_0), \Omega(x_0))]\,, \qquad (3)$$

$a^2(x_0)$ and $\Omega(x_0)$ being functions of x_0, and

$$\tilde{w}_1(x_0, a^2(x_0), \Omega(x_0)) = \frac{1}{\beta} \ln\left[\frac{\sinh(\beta\Omega/2)}{\beta\Omega/2}\right] - \frac{\Omega^2 a^2}{2} + V_{a^2}(x_0)\,, \qquad (4)$$

where Ω is a parameter allowing to define the auxiliary potential $\tilde{w}_1(x_0, a^2(x_0), \Omega(x_0))$ and $V_{a^2}(x_0)$ is the smeared out version of the $V(x)$ potential, defined as

$$V_{a^2}(x_0) = \int \frac{\mathrm{d}x'}{(2\pi a^2)^{1/2}} \exp\left\{-\frac{(x_0-x')^2}{2a^2}\right\} V(x') \qquad (5)$$

with a^2 as an unknown parameter.

The classical limit of the partition function is reached for high temperatures ($T\to\infty$), for which $w(x_0)\to V(x_0)$ and therefore

$$Z \to Z_{\mathrm{cl}} = \int \frac{\mathrm{d}x_0}{(2\pi\beta)^{1/2}} \exp[-\beta V(x_0)]\,. \qquad (6)$$

One may thus say that, because of the analogy with the classical limit $w(x_0)\to V(x_0)$, $w(x_0)$ is the classical effective potential, and that the integral (2) is the classical effective partition function.

A relation between the parameters a^2 and Ω can be established through the minimization of $\tilde{w}_1(x_0, a^2(x_0), \Omega(x_0))$ with respect to Ω. So, for each x_0 we shall obtain the relation

$$a^2 = \frac{1}{\beta\Omega^2}\left[\frac{\beta\Omega}{2}\coth\frac{\beta\Omega}{2} - 1\right]. \qquad (7)$$

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Similarly, the minimization of $\tilde{w}_1(x_0, a^2(x_0), \Omega(x_0))$ with respect to $a^2(x_0)$ allows us to work out $\Omega^2(x_0)$,

$$\Omega^2(x_0) = 2\,\frac{\partial V_{a^2}(x_0)}{\partial a^2} = \frac{\partial^2 V_{a^2}(x_0)}{\partial x_0^2}\,. \tag{8}$$

Equations (3)–(5) have been obtained from the trial partition function Z, the effect of its potential energy on the x_n $(n \neq 0)$ components having been approximated by a Gaussian-potential according to the equation

$$Z_1 \equiv e^{-\beta F_1} = \int \mathscr{D}\, x(\tau) \tag{9}$$

$$\cdot \exp\left\{-\int_0^\beta \mathrm{d}\tau \left\{\frac{\dot{x}^2(\tau)}{2} + \frac{\Omega^2(x_0)}{2}(x(\tau)-x_0)^2\right\} - \beta L_1(x_0)\right\},$$

where $\Omega^2(x_0)$ is a local arbitrary curvature of the potential, and where $L_1(x_0)$ is the trial potential depending only on the x_0 mean coordinate. The $\Omega(x_0)$ and $L_1(x_0)$ functions are determined by the extremal principle. Thus, (9) can be reduced to a simple integral over x_0,

$$Z_1 = \int \frac{\mathrm{d}x_0}{(2\pi\beta)^{1/2}}\;\frac{\beta\,\Omega(x_0)/2}{\sinh\left(\dfrac{\beta\,\Omega(x_0)}{2}\right)}\exp\{-\beta L_1(x_0)\}\,, \tag{10}$$

where L_1 is gven by the relation

$$L_1(x_0) = V_{a^2(x)}(x_0) - \Omega^2(x_0)\,a^2(x_0)/2\,. \tag{11}$$

We can see that (10) and (2) are similar. The example that we wish to work on in this paper is the harmonic oscillator, the family of potentials of which can be obtained through factorization [3].

The following potentials have already been dealt with: the Coulomb potential [6], the anharmonic oscillator [1, 2], the Yukawa potential [1, 2], and the harmonic oscillator plus the Dirac distribution [7].

We shall now apply the Feynman-Kleinert method to a class of harmonic oscillators. These harmonic potentials may be obtained through the following method.

Let us consider the factorized expression

$$H + \tfrac{1}{2} = a\,a^\dagger\,, \tag{12}$$

where H is the Hamiltonian and where $a^\dagger$ and a are respectively the creation and anihilation operators, defined by

$$a = \frac{1}{\sqrt{2}}\left(\frac{\mathrm{d}}{\mathrm{d}x} + x\right), \quad a^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{\mathrm{d}}{\mathrm{d}x} + x\right).$$

Let us define two new operators

$$b = \frac{1}{\sqrt{2}}\left(\frac{\mathrm{d}}{\mathrm{d}x} + \beta(x)\right), \quad b^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{\mathrm{d}}{\mathrm{d}x} + \beta(x)\right), \tag{13}$$

by imposing

$$H + \tfrac{1}{2} = b\,b^\dagger\,, \tag{14}$$

which leads us to

$$-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}x^2 + \frac{1}{2} = \frac{1}{2}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \beta' + \beta^2\right), \tag{15}$$

the condition on β being Ricatti's equation

$$\beta' + \beta^2 = 1 + x^2\,,$$

the solution of which can be obtained by setting

$$\beta = x + \phi(x)\,. \tag{16}$$

Hence, we have

$$\phi(x) = \frac{e^{-x^2}}{\gamma + \int_0^x e^{-x'^2}\,\mathrm{d}x'}\,, \qquad \gamma \in \mathbb{R}\,.$$

The relation between the hamiltonian and modified hamiltonian of the harmonic oscillator can be written

$$H' = H - \phi'(x) = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \tag{17}$$

with

$$V(x) = \frac{x^2}{2} - \frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{e^{-x^2}}{\gamma + \int_0^x e^{-x'^2}\,\mathrm{d}x'}\right]. \tag{18}$$

This potential $V(x)$ can be written

$$V(x) = \frac{x^2}{2} + \sum_{n=1}^{\infty} g_n\,x^n, \quad -\infty < x < \infty\,, \tag{19}$$

with $g_n \to 0$, when $|\gamma| \to +\infty$.

If $|\gamma| > \frac{1}{2}\sqrt{\pi}$, the above potential has no singularity and behaves like $x^2/2$, for $x \to \pm\infty$, and we thus obtain here a one-parameter family of self-adjoint Hamiltonians in $L^2(R)$. It is to be noted that the eigenvalues of H and H' are the same, namely

$$H'\phi_n = (n + \tfrac{1}{2})\,\phi_n\,, \quad (n = 1, 2, 3, \ldots, \infty)\,, \tag{20}$$

whereas the wave functions ψ_n and ϕ_n of the harmonic oscillator and the modified harmonic oscillator, re-

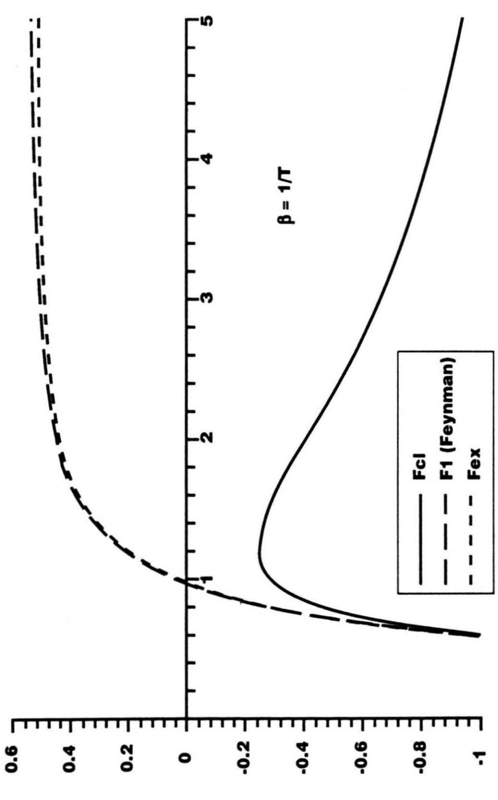

Fig. 1. F_{ex}, F_{cl}, F_1, for $\gamma = 0.9$, versus $\beta = 1/T$.

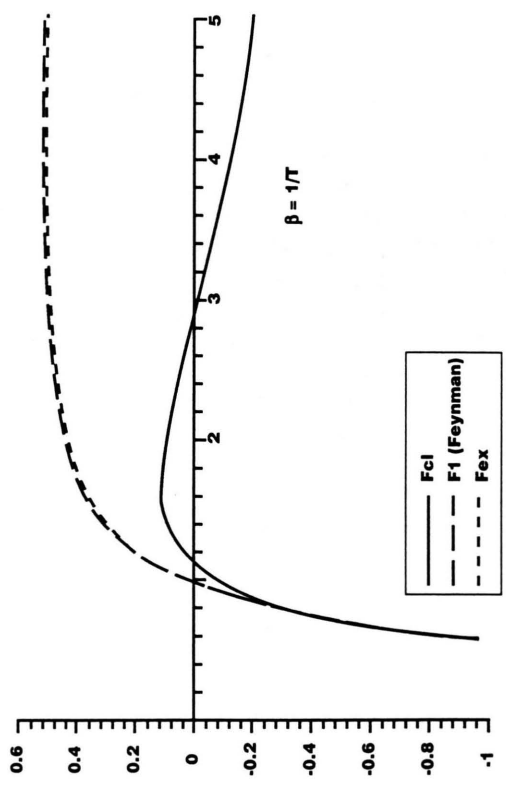

Fig. 2. F_{ex}, F_{cl}, F_1, for $\gamma = 1$, versus $\beta = 1/T$.

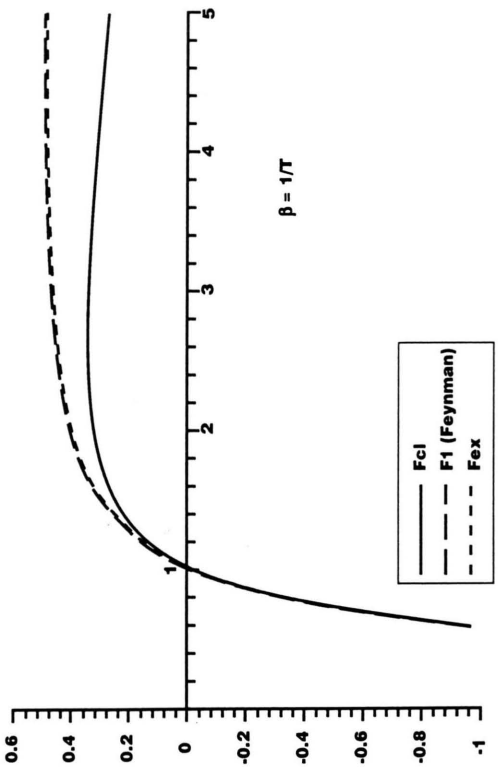

Fig. 3. F_{ex}, F_{cl}, F_1, for $\gamma = 3$, versus $\beta = 1/T$.

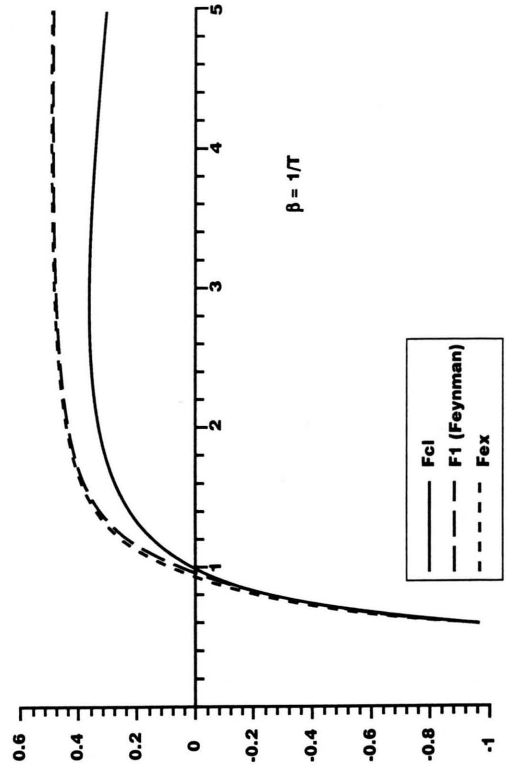

Fig. 4. F_{ex}, F_{cl}, F_1, for $\gamma = 5$, versus $\beta = 1/T$.

Table 1. Comparison of the variational energy $E^0 = \lim_{T \to 0} F_1$, obtained from a Gaussian trial wave function, with the exact energy E^0_{ex} of the ground state. The level-splitting $\Delta E^0_{ex} = E^1_{ex} - E^0_{ex}$ of the first excited state (shown in column 5) is well approximated by the $\Omega(0)$ value.

$\|\gamma\|$	E^0	E^0_{ex}	E^1_{ex}	ΔE^0_{ex}	$\Omega(0)$	$a^2(0)$
0.9	0.5350	0.4950	1.4962	1.0225	0.8895	0.7889
1.0	0.5211	0.4975	1.4975	1.0065	0.8952	0.6455
1.5	0.5088	0.4990	1.4991	1.0031	0.8983	0.5221
2.0	0.5035	0.4996	1.4995	1.0022	0.9350	0.4858
3.0	0.5012	0.4999	1.4999	1.0005	0.9543	0.4832
5.0	0.5006	0.4999	1.4999	1.0002	0.9860	0.4806

spectively, are related by the equation

$$\phi_n = - b^\dagger \psi_{n-1} \,. \tag{21}$$

In particular, for the ground state we have

$$\phi_0 = c_0 \, e^{-x^2/2} \exp\left\{ - \int_0^x \phi(x') \, dx' \right\}. \tag{22}$$

Table 1 allows us to compare the variational energy $E^0 = \lim_{T \to 0} F_1$, obtained for a Gaussian trial wave function, with the exact energy E^0_{ex} of the ground state. The $\Delta E^0_{ex} = E^1_{ex} - E^0_{ex}$ values (fifth column) appear to be in good accordance with $\Omega(0)$, at $T = 0$. Four figures give F_{ex}, F_1 (Feynman) and F_{cl} versus $\beta = 1/T$, for $\gamma = 0.9$, 1.0, 3.0, and 5.0 respectively.

To conclude, we may say that the semi-classical approximation proposed by Feynman-Kleinert [1, 2], when applied to the class of potentials obtained by the factorization method [3], leads to a very good accordance with the exact free energy, for all temperatures. The maximal difference, observed for $|\gamma| = 0.9$, does not exceed 4 per cent. At low temperatures ($\beta > 5$), the semi-classical energy goes to the ground state energy E_0.

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