STATISTICAL PROPERTIES OF A HARMONIC PLUS A DELTA-POTENTIAL

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For a singular but solvable potential we test a new variational approach for calculating statistical properties of quantum systems proposed recently by Feynman and Kleinert. We consider a potential consisting of a sum of a harmonic oscillator and a delta-potential. We solve the Schrödinger equation analytically, calculate exact free energies and particle densities, and compare with the variational approach. We find good agreement in a wide range of temperature and strength of the delta-potential.

1. Introduction

Recently, Feynman and Kleinert [1] [#1] proposed a new variational method for calculating statistical properties of quantum mechanical systems. It is a generalization of a well-known approximation given a long time ago by Feynman [3] to which it reduces for a special, non-optimal choice of the variational parameters. Up to now, it has been used to study free energies and particle densities for the one-dimensional anharmonic oscillator and double-well potential [1,4–6] and to investigate the radial distribution function of the three-dimensional Coulomb problem [7]. In all cases, the new approximation gives reasonably good results even at relatively low temperatures. In this note, we test the method for a much more singular potential: the harmonic oscillator with a delta-potential at the origin. Its accuracy is tested by comparing free energies and particle densities with the exact analytical solution which we derive first.

2. Exact solution

Let us start by studying the quantum mechanics of a somewhat more general potential, namely the bi-harmonic oscillator with a displaced delta-potential. With the oscillator frequency being respectively ω_1 for $y>0$ and ω_2 for $y<0$, the potential is of the form

$$V(y)=\tfrac{1}{2}m[\omega_1^2\Theta(y)+\omega_2^2\Theta(-y)]y^2 + \alpha\delta(y-y_0)\,, \tag{1}$$

where $\Theta(y)$ is the step function, and α and $y_0\geqslant 0$ are the strength and the location of the delta-potential. Introducing dimensionless variables via

$$x\equiv\sqrt{m\omega_1/\hbar}\,y,\quad \omega^2\equiv\omega_2^2/\omega_1^2,\quad E\equiv\hbar\omega_1\epsilon,$$
$$a\equiv\sqrt{m/\hbar^3\omega_1}\,\alpha$$

the Schödinger equation $[(-\hbar^2/2m)\mathrm{d}^2/\mathrm{d}y^2+V(y)]\psi(y)=\epsilon\psi(y)$ becomes

$$-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x)+\{\tfrac{1}{2}[\Theta(x)+\omega^2\Theta(-x)]x^2 + a\delta(x-x_0)\}\psi(x)=E\psi(x)\,. \tag{2}$$

Since the wave functions must vanish as $x\to\pm\infty$, it is easy to show that the solutions of (2) are of the form ($z\equiv\sqrt{2}\,x$)

$$\begin{aligned}\psi(x)&=AD_\nu(-\sqrt{\omega}\,z)\,, & z\leqslant 0\,,\\ &=BD_\mu(z)+CD_\mu(-z)\,, & 0<z\leqslant z_0\,,\\ &=DD_\mu(z)\,, & z_0\leqslant z\,,\end{aligned} \tag{3}$$

with $E=\mu+\frac{1}{2}=\omega(\nu+\frac{1}{2})$. $D_\mu(\ )$ and $D_\nu(\ )$ denote parabolic cylinder functions [8], and the constants

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[#1] For an independent development along similar lines, see ref. [2].

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A, B, C, D have to be determined by the matching conditions at $x=0$ and $x=x_0$. From the continuity of the wave functions at both places, we have

$$AD_\nu(0)-BD_\mu(0)-CD_\mu(0)=0 \tag{4}$$

and

$$BD_\mu(z_0)+CD_\mu(-z_0)-DD_\mu(z_0)=0\,. \tag{5}$$

At $x=0$, also the derivative $\psi' \equiv \mathrm{d}\psi/\mathrm{d}x$ must be continuous. At $x=x_0$, however, the delta-potential enforces a jump $\psi'(x_0^+)-\psi'(x_0^-)=2a\psi(x_0)$. Using these matching conditions for ψ', we obtain

$$A\sqrt{\omega}\,D_\nu'(0)+BD_\mu'(0)-CD_\mu'(0)=0 \tag{6}$$

and

$$BD_\mu'(z_0)-CD_\mu'(-z_0)$$
$$-D[D_\mu'(z_0)-a\sqrt{2}\,D_\mu(z_0)]=0\,, \tag{7}$$

where $D_\lambda'(\xi)$ denotes the derivative of the parabolic cylinder function with respect to the whole argument evaluated at e.g. $\xi=-z_0$. In order to find a non-trivial solution of (4)–(7), the parameters ν and μ must satisfy the relation

$$[D_\mu'(0)D_\nu(0)+\sqrt{\omega}\,D_\mu(0)D_\nu'(0)]$$
$$\times[D_\mu(-z_0)D_\mu'(z_0)+D_\mu(z_0)D_\mu'(-z_0)]$$
$$=a\sqrt{2}\,D_\mu(z_0)\{D_\mu'(0)D_\nu(0)$$
$$\times[D_\mu(-z_0)+D_\mu(z_0)]$$
$$+\sqrt{\omega}D_\mu(0)D_\nu'(0)[D_\mu(-z_0)-D_\mu(z_0)]\}, \tag{8}$$

which determines the energy eigenvalues $E=\mu+\frac{1}{2}=\omega(\nu+\frac{1}{2})$ of the biharmonic oscillator with displaced delta-potential. Using the recurrence relation $D_\lambda'(\xi)=\frac{1}{2}\xi D_\lambda(\xi)-D_{\lambda+1}(\xi)$, it is easy to show that all $D_\lambda'(\;)$ in eq. (8) can be replaced by $-D_{\lambda+1}(\;)$.

Let us now consider some special cases in more detail. In the case of a delta-potential at the origin ($z_0=0$), eq. (8) simplifies to

$$\frac{\sqrt{2}}{2}\left(\frac{D_{\mu+1}(0)}{D_\mu(0)}+\sqrt{\omega}\,\frac{D_{\nu+1}(0)}{D_\nu(0)}\right)=-a\,, \tag{9}$$

with $\frac{1}{2}\sqrt{2}D_{\lambda+1}(0)/D_\lambda(0)=\Gamma(\frac{1}{2}-\frac{1}{2}\lambda)/\Gamma(-\frac{1}{2}\lambda)=-\tan(\frac{1}{2}\pi\lambda)\Gamma(1+\frac{1}{2}\lambda)/\Gamma(\frac{1}{2}+\frac{1}{2}\lambda)$. For $a=0$, i.e. for the biharmonic oscillator *without* delta-potential, this reduces to eq. (7) of ref. [9] as expected.

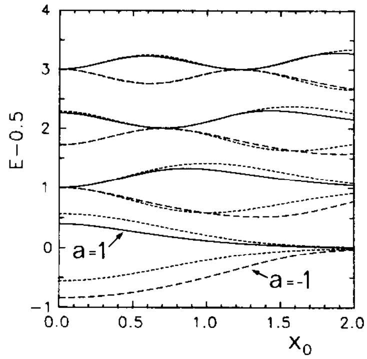

Fig. 1. Energy eigenvalues of the harmonic oscillator ($\omega=1$) with displaced delta-potential versus displacement x_0 in the attractive ($a=-1$, dashed lines) and repulsive ($a=1$, solid lines) case. The short-dashed curves show the energies in first-order perturbation theory.

For later purposes, we concentrate hereafter on the harmonic case $\omega_1=\omega_2$ ($\omega=1$) in which eq. (8) becomes

$$\frac{\sqrt{2}}{2}\left(\frac{D_{\mu+1}(z_0)}{D_\mu(z_0)}+\frac{D_{\mu+1}(-z_0)}{D_\mu(-z_0)}\right)=-a\,, \tag{10}$$

with $E=\mu+\frac{1}{2}$. From (3)–(7) with $\mu=\nu$, we obtain the eigenfunctions [#2] ($z\equiv\sqrt{2}\,x$)

$$\psi(x)=CD_\mu(-z), \qquad z\leqslant z_0,$$
$$=C[D_\mu(-z_0)/D_\mu(z_0)]D_\mu(z), \quad z_0\leqslant z, \tag{11}$$

where the normalization constant is

$$C=\left[\int_{-\infty}^{x_0}\mathrm{d}x\,[D_\mu(-\sqrt{2}\,x)]^2+\left(\frac{D_\mu(-\sqrt{2}\,x_0)}{D_\mu(\sqrt{2}\,x_0)}\right)^2\right.$$
$$\left.\times\int_{x_0}^{\infty}\mathrm{d}x\,[D_\mu(\sqrt{2}\,x)]^2\right]^{-1/2}. \tag{12}$$

The transcendental equation (10) for the energy eigenvalues has to be solved numerically. For $a=\pm 1$, the solutions are shown in fig. 1 where the eigenvalues $E_n=\mu+\frac{1}{2}$ of the the first four states are plotted versus the displacement variable x_0. The short-dashed curves are the energies in first-order perturbation theory, $E_n^{(1)}=n+\frac{1}{2}+a|\phi_n(x_0)|^2$ with $\phi_n(x_0)$ being the well-known harmonic oscillator eigenfunc-

[#2] Eigenfunctions and energies are labeled according to the states of the unperturbed harmonic oscillator.

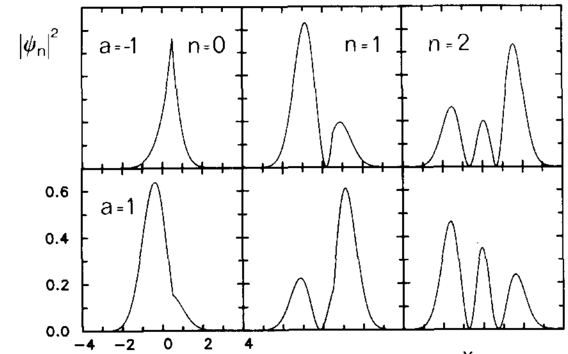

Fig. 2. Probability densities of the first three states of the harmonic oscillator ($\omega=1$) with a delta-potential at $x_0=0.5$ in the attractive ($a=-1$, upper part) and repulsive ($a=1$, lower part) case. In the upper left plot, the vertical scale has to be multiplied by a factor 2.

tions. Note that in case x_0 hits a zero of $\phi_n(x_0)$, the nth energy level of the pure harmonic oscillator is *not* perturbed at all, since then the delta-potential cannot be "felt" by the wave function [#3]. Hence, for $x_0=0$, all *odd* levels are unperturbed. For the delta-potential at $x_0=0.5$, the normalized probability densities $|\psi_n(x)|^2$ of the first three states are displayed in fig. 2 for the attractive ($a=-1$, upper part) and repulsive ($a=1$, lower part) case.

Finally, let us consider the most symmetric situation with the delta-potential being located at the origin. Then, we find from (10) the simple relation

$$\sqrt{2}\frac{D_{\mu+1}(0)}{D_\mu(0)}=2\frac{\Gamma(\frac{1}{2}-\frac{1}{2}\mu)}{\Gamma(-\frac{1}{2}\mu)}-2\tan(\pi\mu/2)\frac{\Gamma(1+\frac{1}{2}\mu)}{\Gamma(\frac{1}{2}+\frac{1}{2}\mu)}=-a \quad (13)$$

for the even energy eigenvalues $E=\mu+\frac{1}{2}$, and the normalized eigenfunctions of the even states are

$$\psi_n(x)=\left(\frac{2}{\sqrt{\pi}}\frac{\Gamma(-\mu)}{\Psi(\frac{1}{2}-\frac{1}{2}\mu)-\Psi(-\frac{1}{2}\mu)}\right)^{1/2}\times D_\mu(\sqrt{2}\,|x|)\,, \quad (14)$$

where $\Psi(\;)=\Gamma'(\;)/\Gamma(\;)$ denotes the logarithmic derivative of the gamma function. As mentioned above, the odd eigenfunctions and eigenvalues are the same as those of the harmonic oscillator. For $a=-1$, -0.5, 0.5, 1, the eigenvalues of the first six even states are given in table 1, and in fig. 3 we show $|\psi_n(x)|^2$ for the first three even states in the attractive ($a=-1$, upper part) and repulsive ($a=1$, lower part) case. As expected, the discontinuities of the derivatives at the origin are clearly visible. We have checked these results by a direct numerical integration of the Schrödinger equation which is straightforward even in the case of a delta-potential at the origin.

Knowing the energies and eigenfunctions from (13) and (14), we can then calculate the exact free energy F from

$$e^{-\beta F}=Z=\sum_n e^{-\beta E_n} \quad (15)$$

[#3] From the non-trivial zeroes of the Hermite polynomials we find for $n=2$: $x_0^{(1)}=\sqrt{1/2}$; $n=3$: $x_0^{(1)}=\sqrt{3/2}$; $n=4$: $x_0^{(1,2)}=\sqrt{[(3\pm\sqrt{6})/2]}=0.5246,\ 1.6507$; $n=5$: $x_0^{(1,2)}=\sqrt{[(5\pm\sqrt{10})/2]}=0.9586, 2.0202$; etc.

Table 1
Energies of even states for a harmonic oscillator plus delta-potential $V(x)=\frac{1}{2}x^2+a\delta(x)$ for various strengths a. The odd states are not affected by the delta-potential.

n	a				
	-1.0	-0.5	0	0.5	1.0
0	-0.3424	0.1556	0.5	0.7335	0.8927
2	2.2208	2.3573	2.5	2.6354	2.7546
4	4.2912	4.3940	4.5	4.6037	4.7002
6	6.3258	6.4118	6.5	6.5870	6.6699
8	8.3473	8.4229	8.5	8.5764	8.6501
10	10.3624	10.4306	10.5	10.5689	10.6359

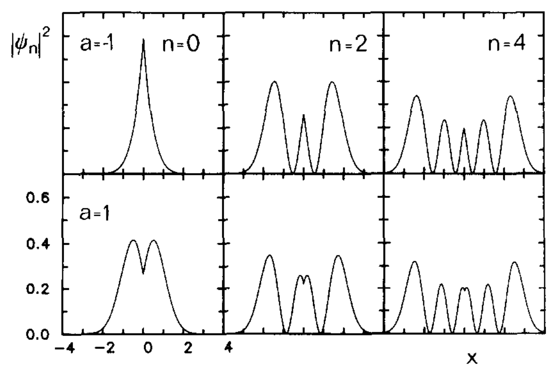

Fig. 3. Probability densities of the first three *even* states of the harmonic oscillator plus delta-potential $V(x)=\frac{1}{2}x^2+a\delta(x)$ in the attractive ($a=-1$, upper part) and repulsive ($a=1$, lower part) case. In the upper left plot, the vertical scale has to be multiplied by a factor 2.

and the exact (normalized) particle distribution function

$$\rho(x) = Z^{-1} \sum_n |\psi_n(x)|^2 \, e^{-\beta E_n} , \tag{16}$$

where $\beta = 1/T$ is the inverse temperature.

3. Feynman–Kleinert method

Let us now come to the main purpose of this note, namely the comparison of these statistical quantities with the Feynman–Kleinert variational approximation [1]. Applied to our case, this method can be summarized as follows:

First, calculate from $V(x) = \frac{1}{2}x^2 + a\delta(x)$ the smeared-out potential

$$V_{\sigma^2}(x) \equiv \int_{-\infty}^{\infty} \frac{dx'}{\sqrt{2\pi\sigma^2}} V(x') \exp\left(-\frac{(x-x')^2}{2\sigma^2}\right)$$

$$= \tfrac{1}{2}(x^2+\sigma^2) + \frac{a}{\sqrt{2\pi\sigma^2}} \exp(-x^2/2\sigma^2) , \tag{17}$$

where

$$\sigma^2 = \frac{1}{\beta\Omega^2} \left(\tfrac{1}{2}\beta\Omega \coth \tfrac{1}{2}\beta\Omega - 1\right) . \tag{18}$$

Second, determine the parameter Ω^2 self-consistently from

$$\Omega^2 = 2 \frac{\partial}{\partial\sigma^2} V_{\sigma^2}(x)$$

$$= 1 - \frac{1}{\sigma^2}\left(1 - \frac{x^2}{\sigma^2}\right) \frac{a}{\sqrt{2\pi\sigma^2}} \exp(-x^2/2\sigma^2) . \tag{19}$$

Third, calculate the effective classical potential

$$W_1(x) = \frac{1}{\beta} \log \frac{\sinh \frac{1}{2}\beta\Omega}{\frac{1}{2}\beta\Omega} - \frac{\Omega^2\sigma^2}{2} + V_{\sigma^2}(x) . \tag{20}$$

An upper bound F_1 [1] for the free energy and the approximate particle density $\rho_1(x)$ [5] are then given by

$$e^{-\beta F_1} = Z_1 = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\beta}} e^{-\beta W_1(x)} \tag{21}$$

and

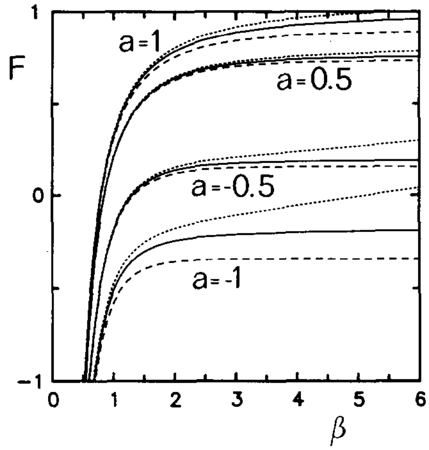

Fig. 4. Free energy for a harmonic oscillator plus delta-potential $V(x) = \frac{1}{2}x^2 + a\delta(x)$ with $a = -1, -0.5, 0.5, 1$. Shown are the exact results (– – –), the Feynman–Kleinert approximation (—) and the original Feynman approximation (- - -).

$$\rho_1(x) = \frac{1}{Z} \int_{-\infty}^{\infty} \frac{dx'}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-x')^2}{2\sigma^2}\right) \times \frac{e^{-\beta W_1}(x')}{\sqrt{2\pi\beta}} . \tag{22}$$

Note that for the non-optimal choice $\Omega^2 = 0$, $\sigma^2 = \beta/12$, one recovers the well-known approximation proposed a long time ago by Feynman [3].

The results of this algorithm are shown in figs. 4 and 5, where we plot free energies and particle densities, respectively. In fig. 4, we compare the exact free energy F from (15) (with $n_{max} = 67$, dashed curves), F_1 from (21) (solid curves) and the original Feynman approximation F_0 ($\Omega^2 = 0$, dotted curves) for various strengths of the delta-potential. We see that $F \leqslant F_1 \leqslant F_0$ as we expect from the variational principle. At higher temperature (up to $\beta \approx 1$), F and F_1 are in exellent agreement. For $a \leqslant |0.5|$, we have very good results even up to $\beta \approx 6$. The worst case shown is $a = -1$ and $\beta = 6$ where the Feynman–Kleinert approximation is $\approx 30\%$ off. Obviously, in all cases, the new method gives much improved results with respect to the original approximation [#4].

[#4] This can be seen most clearly in the limit $T \to 0$ where the original method is completely off, whereas the new method gives at least reasonable results.

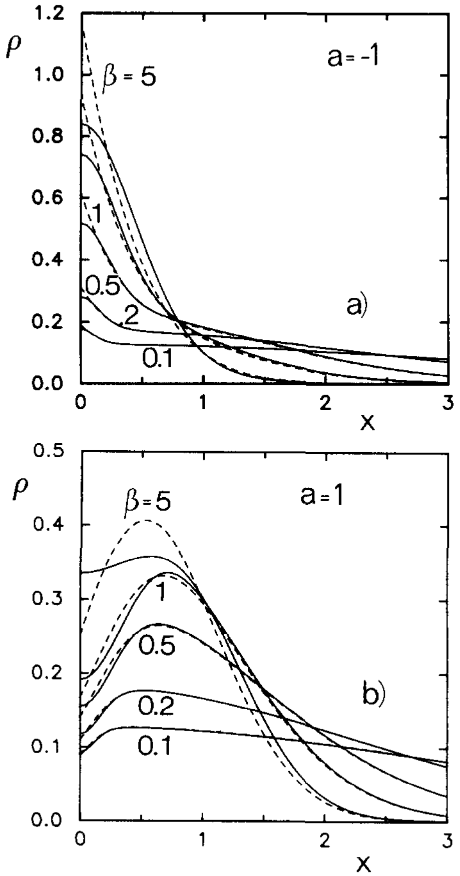

Fig. 5. Normalized particle density for a harmonic oscillator plus delta-potential $V(x)=\frac{1}{2}x^2+a\delta(x)$ at various temperatures $T=1/\beta$ in (a) the attractive ($a=-1$) and (b) repulsive ($a=1$) case. Compared are the exact results (- - -) and the Feynman–Kleinert approximation (—).

In fig. 5, we compare the exact particle densities from (16) (with $n_{max}=51$, dashed curves) with the Feynman–Kleinert approximation (22) (solid curves) for $a=\pm 1$ and various temperatures $T=1/\beta$. At higher temperatures $\beta \leqslant 0.2$, the approximation is excellent in the whole range of x. For intermediate temperatures $0.5 \leqslant \beta \leqslant 1$, there are small deviations near the location of the delta-potential, i.e. for $|x| \leqslant 0.5$. Only for very low temperatures $\beta \geqslant 5$ and small $|x| \leqslant 1$, the Feynman–Kleinert approximation is no longer reliable.

4. Discussion

In this note, we have shown by comparison with exact results that the Feynman–Kleinert method can be applied even to singular potentials with reasonable accuracy. In the particular example of the harmonic oscillator plus a delta-potential, the smeared-out potential is of the smooth gaussian type. While preparing our manuscript, we found ref. [10] in which the harmonic osillator with a delta-potential at the origin was also studied analytically, albeit with a completely different motivation. As a final remark, we would like to point out a printing error in their eq. (12) (a factor $2\sqrt{2}$ is missing on the right-hand side) and that their fig. 1 is correct at best schematically.

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