CHAPTER VI

DETAILED DISCUSSION AND CONCLUSION

The expected accuracy of the approximate effective classical potential given by Feynman and Kleinert approach can be assessed by the following observation: In the limit of high temperatures, the accuracy is perfect both for the approximate effective classical potential and its approximation $W_1(x_0)$ which tend correctly to the classical potential $V(x_0)$. In the opposite limit of low temperatures, the integral over x_0 in (5.50) will be dominated by the minimum of $W_1(x_0)$. By taking the $T \to 0$ limit in (5.51) we see that

$$\lim_{T \to 0} W_1(x_0) = \frac{1}{2}\left[\hbar\Omega(x_0) - M\Omega^2(x_0)a^2(x_0)\right] + V_{a^2(x_0)}(x_0). \qquad (6.1)$$

In the same limit, (5.56) gives

$$\lim_{T \to 0} a^2(x_0) = \frac{\hbar}{2M\Omega(x_0)}, \qquad (6.2)$$

so that

$$\lim_{T \to 0} W_1(x_0) = \left[\frac{3}{4}\hbar\Omega(x_0) + V_{a^2(x_0)}(x_0)\right] = \left[\frac{3}{8}\frac{\hbar^2}{Ma^2(x_0)} + V_{a^2(x_0)}(x_0)\right], \qquad (6.3)$$

to be minimized in $a(x_0)$. The integral in (5.50) is dominated by the minimum of this with respect to x_0. But the right-hand side of (6.3) is recognized to be simply the expectation value of the Hamiltonian operator,

$$\hat{H} = \frac{\hat{p}^2}{2M} + V(x), \qquad (6.4)$$

in a normalized Gaussian wave packet of width a centered at x_0,

$$\psi(x) \;=\; \frac{1}{2\pi a^2} \exp\left\{-\frac{a^2}{2}(x - x_0)^2\right\}. \tag{6.5}$$

Indeed,

$$\left\langle \hat{H} \right\rangle_\psi \;\equiv\; \int_{-\infty}^{\infty} dx\, \psi^*(x)\hat{H}\psi(x) \;=\; \frac{3}{8}\frac{\hbar^2}{Ma^2} + V_{a^2}(x_0). \tag{6.6}$$

Let E_1 be the minimum of this expectation under variation of x_0 and a^2,

$$E_1 \;=\; \min_{x_0,\, a^2} \left\langle \widehat{H} \right\rangle_\psi . \tag{6.7}$$

Then what we have just shown is that

$$\lim_{T \to 0} F_1 \;=\; E_1 . \tag{6.8}$$

In the low-temperature limit, the exact free energy tends to the exact ground state energy E_0. The quality of the approximate effective classical potential $W_1(x_0)$ in the low-temperature limit is therefore as good as the estimate for the ground state energy E_0 rendered by the minimal expectation value E_1 of the Hamiltonian operator in a Gaussian wave packet. For potentials with a pronounced unique minimum of quadratic shape this estimate is known to be excellent.

For the application to anharmonic oscillator of the potential $V(x) = x^2/2 + gx^4/4$ now we use $M = \hbar = k_B = 1$ again, the approximate free energies $F_1 = 1/\beta \ln Z_1$ are plotted as a function of β in Fig. 6.1.

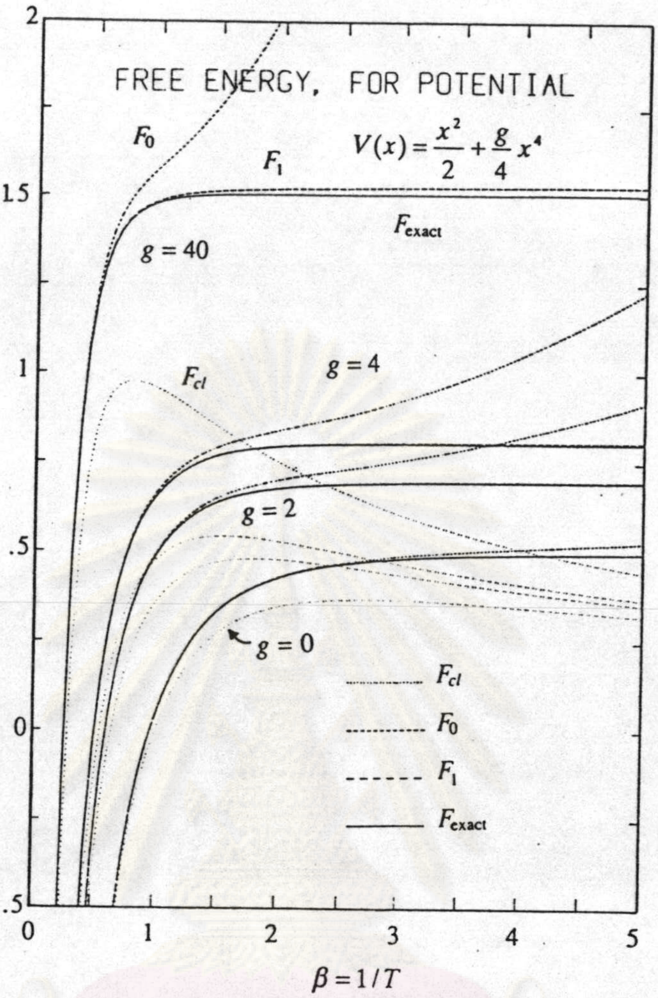

Figure 6.1 The approximate free energy F_1 of the anharmonic oscillator as compared with the exact one, F_{ex}, the classical one $F_{cl} = -(1/\beta) \ln \int \left(dx / \sqrt{2\pi\beta}\right) \times e^{-\beta V(x)}$, and as well as and earlier approximation $F_0 = -(1/\beta) \ln Z_0$ given by Feynman in his book on statistical mechanics, which corresponds to F_1 for the non-minimal choice $\Omega = 0, a^2 = \beta / 12$. Notice that F_0, F_1 satisfy the inequality $F_1 \geq F$ while F_{cl} does not[Feynman and Kleinert 1986].

The exact free energy curve calculated from the known energy eigenvalues of the anharmonic oscillator is seen to lie only little below the approximate F_1 curve. For the comparison we have also plotted the classical approximation $F_{cl} = -(1/\beta) \ln Z_{cl}$, which does not satisfy the Jensen-Peierls in equality and lies below the exact curve. In Chapter IV we give earlier Feynman variational, he gives another approximation, here to be called F_0, which can be obtained from the present one by stopping the iteration of (5.66), (5.67) after the first step, i.e., by using the constant non-minimal variational parameters $\Omega \equiv 0, a^2 \equiv \beta/12$ for all x_0. Then $V_{a^2}(x) = V(x) + (\hbar^2\beta/24M) V''(x)$, as in Wigner's expansion[Hillary et. al., 1984]. This approximation is good only at higher temperature. It is also plotted in Fig. 6.1. Just as the curve F_1, it lies above the exact curve since it is also subject to the Jensen-Peierls inequality, which certainly holds for the free energy F_1 with the potential $W_1(x_0)$ in the general form (5.51), i.e., before minimization in a^2 when $\Omega^2(x_0)$ is still arbitrary, in particular for $\Omega^2(x_0) \equiv 0$.

In Table 6.1 we have listed the energies E_1 for an anharmonic potential of various coupling strengths and compared them with precise numerical ground state energies. With the effective classical potential having good high and low-temperature limits it is no surprise that the approximation is quite reliable at all temperatures.

$g/4$	E_1	E^0_{ex}	E^1_{ex}	E^2_{ex}	ΔE^0_{ex}	$\Omega(0)$	$a^2(0)$
0.1	0.5603	0.559146	1.76950	3.13862	1.21035	1.222	0.4094
0.2	0.6049	0.602405	1.95054	3.53630	1.34810	1.370	0.3650
0.3	0.6416	0.637992	2.09464	3.84478	1.45665	1.487	0.3363
0.4	0.6734	0.668773	2.21693	4.10284	1.54816	1.585	0.3154
0.5	0.7017	0.606176	2.32441	4.32752	1.62823	1.627	0.2991
0.6	0.7273	0.721039	2.42102	4.52812	1.69998	1.749	0.2859
0.7	0.7509	0.743904	2.50923	4.71033	1.76533	1.819	0.2749
0.8	0.7721	0.765144	2.59070	4.87793	1.82556	1.884	0.2654

0.9	0.7932	0.785032	2.66663	5.03360	1.86286	1.944	0.2572
1.0	0.8125	0.803771	2.73789	5.17929	1.93412	2.000	0.2500
10	1.5313	1.50497	5.32161	10.3471	3.81694	4.000	0.1250
50	2.5476	2.49971	8.91510	17.4370	6.41339	6.744	0.0741
100	3.1924	3.13138	11.1873	21.9069	8.05590	8.474	0.0590
500	5.4258	5.31989	19.0434	37.3407	13.7235	14.446	0.0346
1000	6.8279	6.69422	23.9722	47.0173	17.2780	18.190	0.0275

Table 6.1 Comparison of the variational energy $E_1 = \lim_{T\to 0}F_1$, obtained from a Gaussian trial wave function with the exact ground state energy $E^0_{\rm ex}$. We also have listed the energy of the first two excited states $E^1_{\rm ex}$ and $E^2_{\rm ex}$. The level splitting $\Delta E^0_{\rm ex} = E^1_{\rm ex} - E^0_{\rm ex}$ to the first excited state is shown in column 6. We see that it is well approximated by the value of $\Omega(0)$, as it should[Kleinert 1990].

For another case of anharmonic oscillator, i.e., double well potential, with the potential $V(x) = -x^2/2 + gx^4/4$ the resulting effective classical potential, and the free energies are plotted in Fig. 6.2, 6.3 and 6.4. It is useful to compare the approximate effective classical potential $W_1(x)$ with the true one $V_{eff,\,cl}(x)$. For this purpose Kleinert performed Monte Carlo simulations of the path integral of the double-well potential with the constraint $x_0 = (1/\beta)\int d\tau\, x(\tau) \equiv$ fixed and extract from these $V_{eff,\,cl}$. We have taken the coupling strength $g = 0.4$, where we expect the agreement to be about the worst. The comparison is shown in Fig. 6.3.

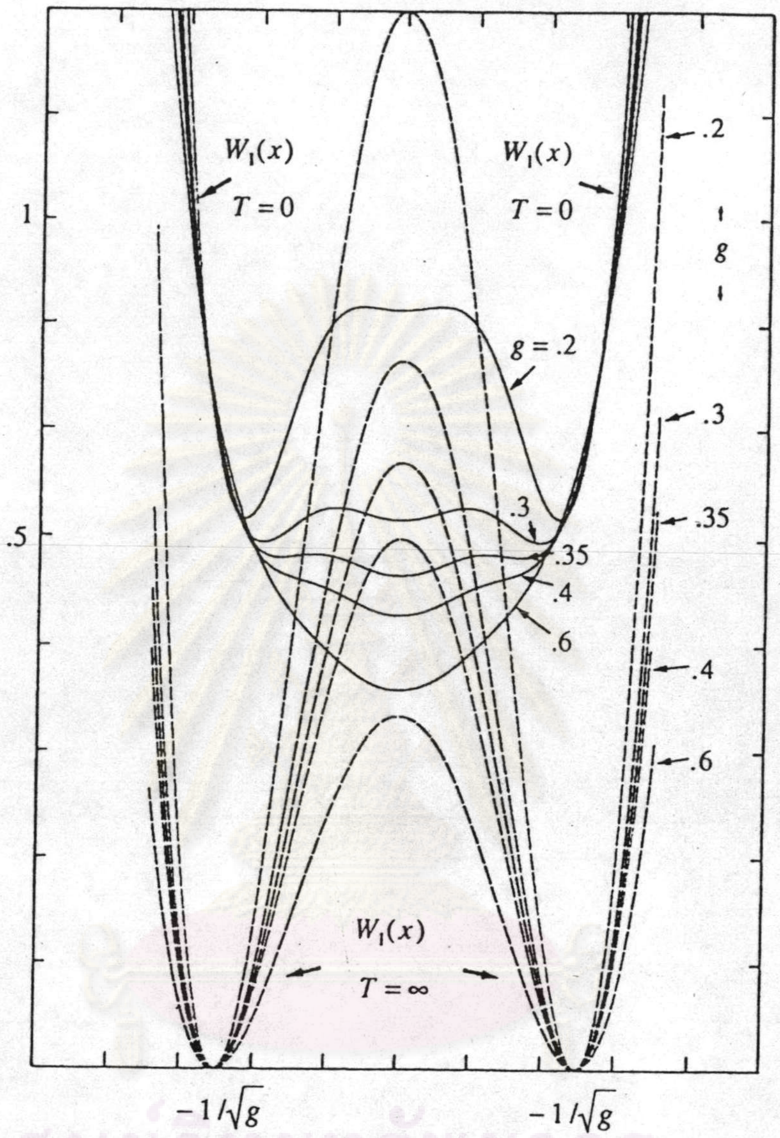

Figure 6.2 The effective classical potential for the double-well $V(x) = -x^2/2 + gx^4/4$ at $T = 0$ and $T = \infty$ where it is equal to the potential $V(x)$ itself. The quantum fluctuations at $T = 0$ smear out the double-well completely if $g = 0.4$, but not if $g = 0.6$[Feynman and Kleinert 1986].

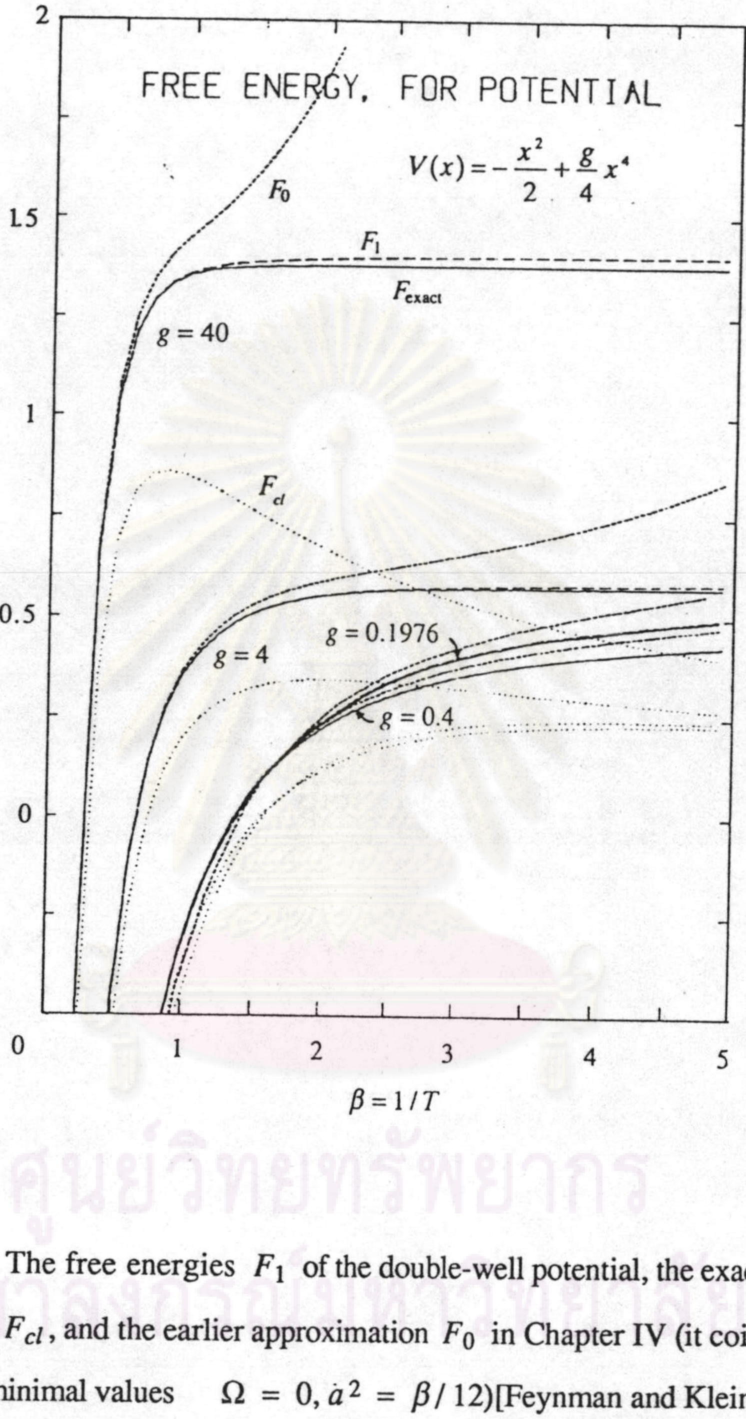

Figure 6.3 The free energies F_1 of the double-well potential, the exact one F_{ex}, the classical one F_{cl}, and the earlier approximation F_0 in Chapter IV (it coincides with F_1 for the non-minimal values $\Omega = 0, a^2 = \beta/12$)[Feynman and Kleinert 1986].

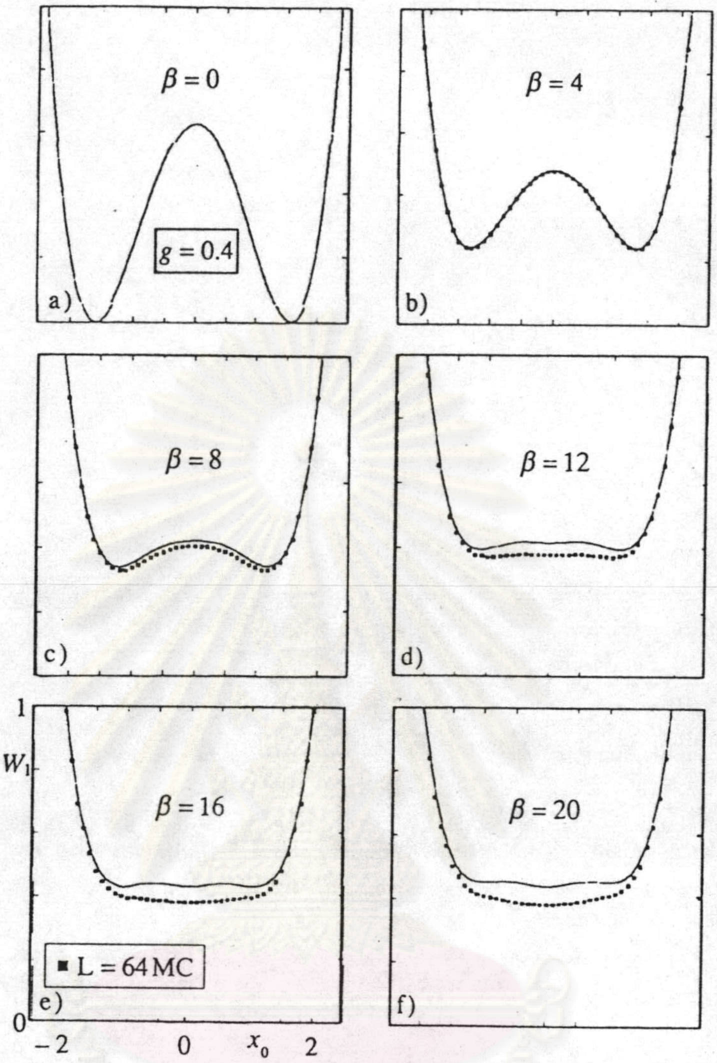

Figure 6.4 Comparison of approximate effective classical potential $W_1(x_0)$ at various inverse temperatures $\beta = 1/T$ with the exact one $V_{eff,\,cl}(x_0)$ as obtained numerically via Monte Carlo simulations based on averages over 10^5 configurations. the data points are from[Janke and Kleinert 1987]. We have picked the worst case $g = 0.4$. The deviations are visible only for $T = 1/\beta \leq 1/8$[Janke and Kleinert 1987].

The new improved variational treatment by Kleinert shown in Chapter V and given the resulting approximation of the partition $Z_3 = e^{-\beta W_3}$ is shown in Fig. 6.5.

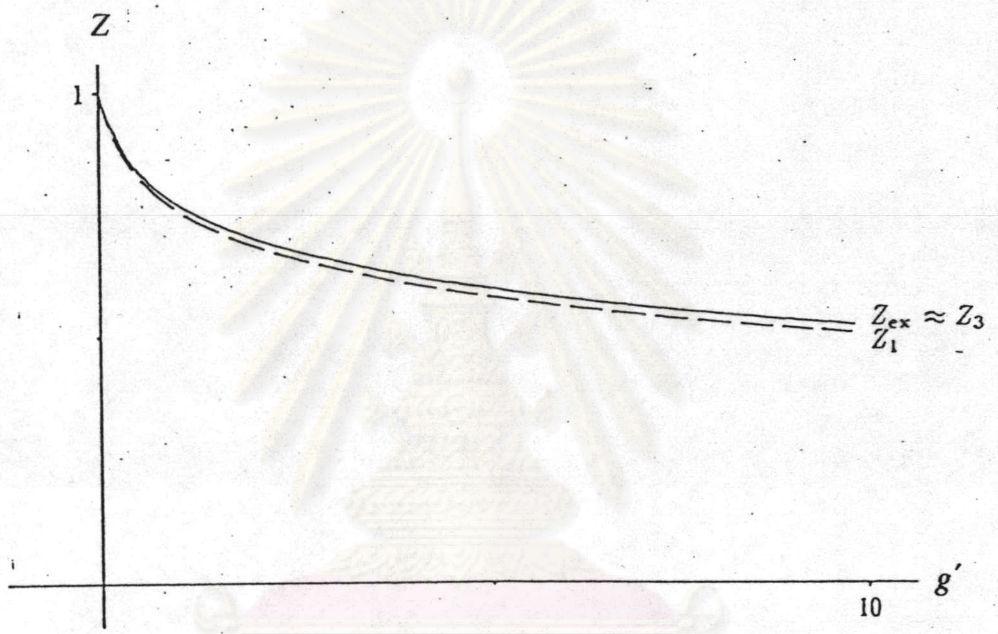

Figure 6.5 The anharmonic model integral as a function of $g' = g / \beta\omega^4$ in comparison with the three variational approximations, Z_1 (dashed) based on the Jensen-Peierls inequality, the new variational approximation Z_3, and the exact Z_{exact}. On this plot, Z_3 lying less than 0.1% below Z_{exact} at $g' = 10$[Kleinert 1993].

The curve lies so closely underneath the exact curve that it is impossible to distinguish the two without magnification. We therefore state the values in Table. 6.2.

The error is everywhere less than .1% amounting to an improvement in accuracy of about a factor 40 with respect to the Feynman-Kleinert approximation.

Note that it is necessary to go to Z_3 to get a substantial improvement over the Feynman-Kleinert approximation Z_1. If we were to stop the expansion in (5.80) after the quadratic terms there would be no extremum in Ω. The reason in the alternating sign of any additional expectations in (5.103) which causes the trial energy of order n to diverge to $(-1)^{n-1} \times \infty$ for $\Omega \to 0$. Since it goes to positive infinity for large Ω, only the odd orders have minima. The even approximations can, however, serve to slightly improve the Feynman-Kleinert by evaluating then at the extremal Ω of the lower odd approximation, as illustrated in the last column of Table 6.2.

g'	Z_{ex}	Z_1	Z_3	Z_2
1	0.772052178	0.759099639	0.771784848	0.779618732
2	0.697727989	0.682058752	0.697379209	0.707793821
3	0.652511915	0.635812008	0.652129205	0.663692090
4	0.620282560	0.603115125	0.619882812	0.632059224
5	0.595411433	0.578026028	0.595002455	0.607536290
6	0.575265822	0.557790484	0.574851763	0.587602248
7	0.558403061	0.540909512	0.557986336	0.570868994
8	0.543948145	0.526478854	0.543530246	0.556491231
9	0.531331175	0.513912161	0.530913086	0.543916527
10	0.520160764	0.502808246	0.519743112	0.532764372

Table 6.2 The new approximation Z_3 for the model partition function (33) as compared with the exact one Z_{ex}, the Feynman-Kleinert approximation Z_1, and the lower-order approximation Z_2[Kleinert 1993].

The minimization of W_3 of (5.80) with respect to Ω give the result shown in Table 6.3

$g'/4$	E_{ex}^0	E_1^0	E_3^0	E_2^0
0.1	0.559146	0.560307371	0.559154219	0.558926659
0.2	0.602405	0.604900748	0.602430628	0.601789378
0.3	0.637992	0.641629862	0.638035761	0.636984919
0.4	0.668773	0.673394715	0.668834137	0.667405766
0.5	0.696176	0.701661643	0.696253638	0.694480729
0.6	0.721039	0.727295668	0.721131779	0.719043542
0.7	0.743904	0.750857818	0.744010403	0.741631780
0.8	0.765144	0.772736359	0.765263715	0.762616228
0.9	0.785032	0.793213066	0.785163496	0.782265430
1	0.803771	0.812500000	0.803914055	0.800781250
10	1.50497	1.53125000	1.50549935	1.49462891
50	2.49971	2.54758040	2.50070646	2.48038428
100	3.13138	3.19244404	3.13265657	3.10661623
500	5.31989	5.42575605	5.32225950	5.27671970
1000	6.69422	6.82795331	6.69722906	6.63962245

Table 6.3 The new approximation E_3^0 for the ground state energy of the anharmonic oscillator (in units $\hbar\omega$) for various couplings g as compared with the exact one E_{ex}^0, the Feynman-Kleinert approximation E_1^0, and the lower order approximation E_2^0 [Kleinert 1993].

The gain in accuracy over the Feynman-Kleinert approximation is also here considerable (about a factor 40). the error is now less than 0.1%. Also shown are the numbers for the even approximation W_2 evaluated at the extremal Ω values of W_1.

In the two examples the new approximate energies always lie above the true ones (a fact which is not true for the even approximations such as W_2). We therefore conjecture that it may be possible to prove an inequality for all odd approximations W_3, W_5, . . . generalizing and sharpening the Jensen-Peierls inequality.