THE EFFECTIVE CLASSICAL POTENTIAL OF THE DOUBLE-WELL POTENTIAL

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We calculate the "effective classical potential" via Monte Carlo simulation and study the accuracy of a recently proposed approximation for it. The approximation is found to be excellent down to very low temperatures $T \gtrsim 1/10$.

The effective classical potential $W(x_0)$ of a quantum system is defined by [1]

$$\exp[-\beta W(x_0)] = (2\pi\beta)^{1/2} \int_{x(0)=x(\beta)} Dx\,\delta\left(x_0 - \frac{1}{\beta}\int_0^\beta d\tau\, x(\tau)\right) \times \exp\left(-\int_0^\beta d\tau\,[\tfrac{1}{2}\dot{x}^2 + V(x(\tau))]\right). \quad (1)$$

The name derives from the fact that in terms of $W(x_0)$, the partition function takes the classical form of a simple integral

$$Z = \int \frac{dx_0}{(2\pi\beta)^{1/2}} \exp[-\beta W(x_0)]\,. \quad (2)$$

For infinite temperature, $W(x_0) = V(x_0)$. The reason for introducing this quantity is that at finite temperature, the fluctuations in x_0 are the most dramatic ones while the deviations from x_0 are sufficiently damped by the kinetic term $\int_0^\beta d\tau\,\frac{1}{2}\dot{x}^2$ such as to be accessible to self-consistent harmonic approximations [1].

If the time axis is sliced into L pieces $\tau_l = \epsilon l$, $l = 1, \ldots, L$, of width $\epsilon = \beta/L$, we expand the periodic paths $x(\tau)$ into a Fourier series

$$x(\tau_l) = x_0 + \frac{1}{L^{1/2}} \sum_{n=1}^{L-1} x_n \exp(i\omega_n \tau_l)\,, \quad (3)$$

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where $\omega_n = (2\pi/\beta)n$ are the Matsubara frequencies and

$$x_n^* = x_{L-n}\,. \quad (4)$$

Thus, all $x_{n\neq 0}$ are complex except for $x_{L/2}$ for even L, which is real. The mode $x_{L/2}$ is associated with the alternating representation $\exp(i\pi l)$ and requires an extra normalization factor. On the lattice, the kinetic term reads

$$\tfrac{1}{2}\int_0^\beta d\tau\,\dot{x}^2 \to \tfrac{1}{2}\epsilon \sum_{l=1}^{L}\left(\frac{x_l - x_{l-1}}{\epsilon}\right)^2 = \tfrac{1}{2}\epsilon \sum_{n=1}^{L-1} \frac{2-2\cos(\omega_n\epsilon)}{\epsilon^2}|x_n|^2\,. \quad (5)$$

Due to (4), each x_n appears twice, except for the real case L=even, $x_{L/2}$. Thus, if we introduce real components $x_n = 2^{-1/2}(x_n^{(1)} + i x_n^{(2)})$, $x_{L/2} = x_{L/2}^{(1)}$, we can write

$$\tfrac{1}{2}\int_0^\beta d\tau\,\dot{x}^2 \to \tfrac{1}{2}\epsilon \sum_{n=1}^{L-1} \frac{2-2\cos(\omega_n\epsilon)}{\epsilon^2}\,\tfrac{1}{2}(x_n^{(1)2} + x_n^{(2)2})\,, \quad (6)$$

where $x_n^{(1),(2)} = \pm x_{L-n}^{(1),(2)}$.

The measure of path integration for finite L is given by

$$\int Dx = \prod_{l=1}^{L}\int_{-\infty}^{\infty} \frac{dx_l}{(2\pi\epsilon)^{1/2}} = \int_{-\infty}^{\infty} \frac{dx_0 L^{1/2}}{(2\pi\epsilon)^{1/2}} \prod_{n=1}^{[\frac{1}{2}L]} \int_{-\infty}^{\infty} \frac{dx_n^{(1)}}{(2\pi\epsilon)^{1/2}} \frac{dx_n^{(2)}}{(2\pi\epsilon)^{1/2}} \quad (7)$$

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with $[\frac{1}{2}L]=$ integer division and $\mathrm{d}x_{L/2}^{\{2\}}$ being absent for $L=$even. For a free particle

$$\exp[-\beta W(x_0)] = L\left(\prod_{n=1}^{L-1}[2-2\cos(\omega_n\epsilon)]^{1/2}\right)^{-1} = 1\,. \tag{8}$$

For a harmonic oscillator with $V=\frac{1}{2}\Omega^2x^2$ we expand

$$\int_0^\beta \mathrm{d}\tau\, V(x(\tau)) = \tfrac{1}{2}\beta\Omega^2x_0^2 + \epsilon\sum_{n=1}^{L-1}\tfrac{1}{2}\Omega^2|x_n|^2 \tag{9}$$

and find

$$\exp[-\beta W(x_0)]$$

$$= L\prod_{n=1}^{L-1}[2-2\cos(\omega_n\epsilon)+\epsilon^2\Omega^2]^{-1/2} \times\exp(-\tfrac{1}{2}\beta\Omega^2x_0^2) \tag{10}$$

$$= L\frac{\frac{1}{2}\epsilon\Omega}{\mathrm{sh}(\frac{1}{2}\beta\Omega_L)}\exp(-\tfrac{1}{2}\beta\Omega^2x_0^2)$$

$$= \frac{\frac{1}{2}\beta\Omega}{\mathrm{sh}(\frac{1}{2}\beta\Omega_L)}\exp(-\tfrac{1}{2}\beta\Omega^2x_0^2)\,, \tag{11}$$

where Ω_L is given by

$$\mathrm{sh}(\tfrac{1}{2}\epsilon\,\Omega_L) \equiv \tfrac{1}{2}\epsilon\Omega\,. \tag{12}$$

For low temperature

$$W(0) = \frac{1}{\beta}\log\left(\frac{\mathrm{sh}(\frac{1}{2}\beta\Omega_L)}{\frac{1}{2}\beta\Omega}\right) \xrightarrow[\beta\to\infty]{} \tfrac{1}{2}\Omega_L \tag{13}$$

giving the zero point energy of the oscillator on a sliced time lattice which reduces to the well-known result $\frac{1}{2}\Omega$ in the limit $L\to\infty$ (i.e. zero width of the spacing).

For an arbitrary potential $V(x)$, the effective classical partition function cannot be found exactly. Still, the harmonic damping of the $n\neq 0$ integrals makes it possible to treat those integrals quite well via a self-consistent harmonic approximation [1] and the result is

$$W(x_0) \leqslant W_1(x_0)$$

$$= \frac{1}{\beta}\log\left(\frac{\mathrm{sh}(\frac{1}{2}\beta\Omega_L)}{\frac{1}{2}\beta\Omega}\right) + V_{a_L^2} - \tfrac{1}{2}\Omega^2a_L^2\,, \tag{14}$$

where

$$a_L^2 = \frac{1}{\beta}\sum_{n=1}^{L-1}\frac{\epsilon^2}{2-2\cos(\omega_n\epsilon)+\epsilon^2\Omega^2}$$

$$= \frac{1}{\Omega}\frac{\partial}{\partial\Omega}\frac{1}{\beta}\log\left(\frac{\mathrm{sh}(\frac{1}{2}\beta\Omega_L)}{\frac{1}{2}\beta\Omega}\right)$$

$$= \frac{1}{\beta\Omega^2}\left(\tfrac{1}{2}\beta\Omega\,\mathrm{cth}(\tfrac{1}{2}\beta\Omega_L)\frac{1}{\mathrm{ch}(\frac{1}{2}\epsilon\Omega_L)} - 1\right), \tag{15}$$

$$\Omega^2 = \frac{\partial^2}{\partial x^2}V_{a_L^2}(x_0)\,, \tag{16}$$

and $V_{a_L^2}(x_0)$ is the potential $V(x_0)$ smeared out by a Gaussian of width a_L^2,

$$V_{a_L^2}(x_0) = \int_{-\infty}^{\infty}\frac{\mathrm{d}x}{(2\pi a_L^2)^{1/2}} \times\exp\left(-\frac{1}{2a_L^2}(x_0-x)^2\right). \tag{17}$$

The purpose of this note is to study how accurately $W_1(x_0)$ approximates the exact effective classical potential $W(x_0)$ for the case of a double-well potential

$$V(x) = -\tfrac{1}{2}x^2 + \tfrac{1}{4}gx^4 \tag{18}$$

for the (about most difficult) case $g=0.4$. This value is large enough to allow for appreciable quantum tunneling (which could be ignored for $g\lesssim 0.1$, say) but not so large that the central barrier can be neglected (as it would be for $g\approx 40$, say). In previous notes we have shown that the approximate $W_1(x_0)$ leads to reliable particle distributions [2] and magnetization curves [3] (i.e. classical potentials of the conventional type, in particular, the classical potential is always convex, due to the final x_0 integration in (2)). Here we want to study $W(x_0)$ itself.

In order to do so we have evaluated the path integral (1) (with sliced time axis) numerically. In momentum space the non-local constraint $\beta^{-1}\int_0^\beta x(\tau)\,\mathrm{d}\tau = x_0$ becomes trivial and (1) can be written as an average over a Gaussian distribution

$$\exp[-\beta W(x_0)]$$

$$= L \prod_{n=1}^{[\frac{1}{2}L]} \int_{-\infty}^{\infty} \frac{dx_n^{(1)}}{(2\pi\epsilon)^{1/2}} \frac{dx_n^{(2)}}{(2\pi\epsilon)^{1/2}}$$

$$\times \exp\left(- \sum_{n=1}^{[\frac{1}{2}L]} \frac{x_n^{(1)2} + x_n^{(2)2}}{2\sigma_n^2} \right)$$

$$\times \exp\left[-\epsilon \sum_{l=1}^{L} V\left(x_0 + \frac{1}{L^{1/2}} \sum_{n=1}^{L-1} x_n \exp(i\omega_n \tau_l) \right) \right]$$

$$\equiv \left\langle \exp\left[-\epsilon \sum_{l=1}^{L} V\left(x_0 + \frac{1}{L^{1/2}} \sum_{n=1}^{L-1} x_n \exp(i\omega_n \tau_l) \right) \right] \right\rangle \tag{19}$$

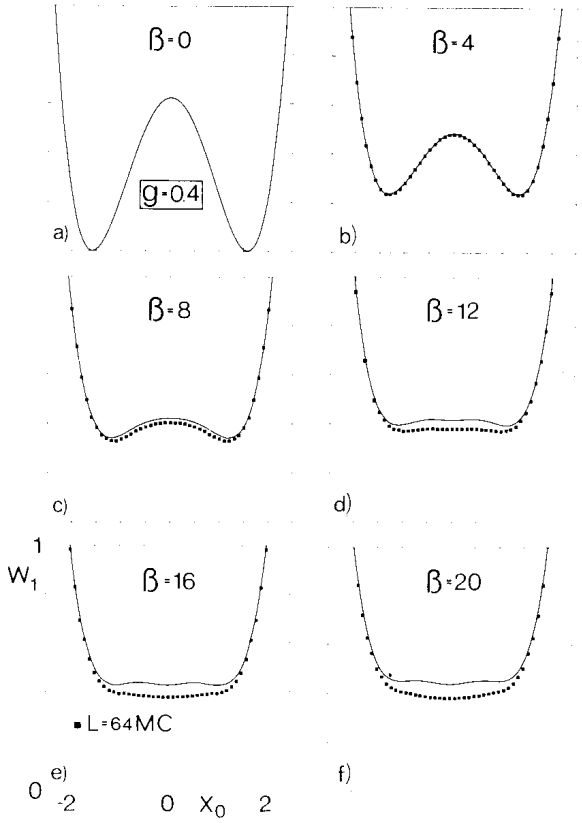

Fig. 1. Comparison of the Monte Carlo data for the effective classical potential $W(x_0)$(■) and the variational bound $W_1(x_0)$ (continuous line) for the double-well potential with $g=0.4$ at various temperatures $T=1/\beta$. The Monte Carlo data are averages over 100000 configurations on a discretized time axis with $L=64$ slices. The error bars are so small that they are completely covered by the data symbols.

with partial variances $\sigma_n^2 = \epsilon/[2-2\cos(\omega_n \epsilon)]$. Recalling the free particle result (8) we see that the average is properly normalized, i.e. $\langle 1 \rangle = 1$. Since Gaussian random numbers are very easy to generate (via $g_1 = (-2 \ln \xi_1)^{1/2} \cos(2\pi\xi_2)$; $g_2 = (-2 \ln \xi_1)^{1/2} \times \sin(2\pi\xi_2)$; $\xi_1, \xi_2 \in (0,1]$) it is straightforward to evaluate this $(L-1)$-dimensional integral via the Monte Carlo method. Given a set of $L-1$ random x_n, most of the computing time is spent in calculating the Fourier transform. Naively, this would require $\approx L^2$ operations. We circumvent this problem by applying the fast-Fourier transform technique, which needs only $\approx L \log L$ operations ‡.

The data shown in figs. 1 and 2 are averages over 100000 Gaussian distributions. With these statistics, all error bars are so small that they are completely covered by the data symbols. Note that *no* equilib-

‡ Optimal time-saving is achieved by choosing $L=2^K$, which explains our choice $L=2, 4, 8, 16, 32, 64$.

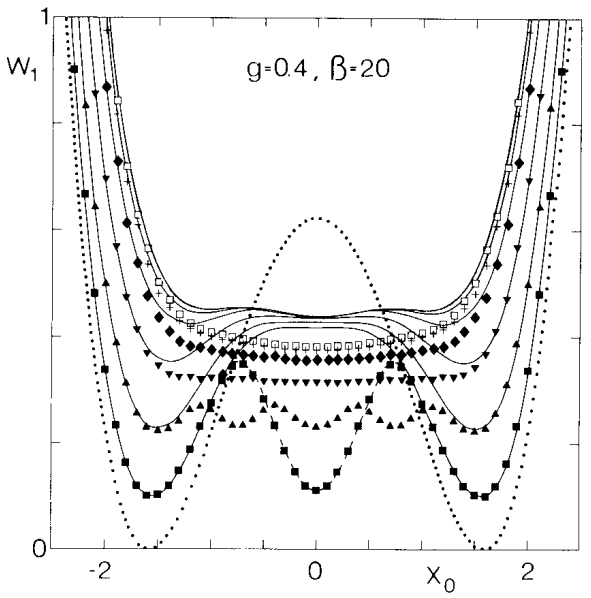

Fig. 2. The effective classical potential of the double-well potential with $g=0.4$ at low temperature as a function of the number of time slices $L=2$ (■), 4(▲), 8(▼), 16(◆), 32 (+) and 64 (□). The continuous lines show the corresponding variational bounds for finite L. The dotted line is the classical potential $V(x_0)$ (corresponding to $L=1$) and the dashed line for $L=2$ is the result of a direct numerical integration. The Monte Carlo data are averages over 100000 configurations.

rium time is needed and that the measurements are *not* affected by unwanted time correlations (assuming that any standard random generator produces at any time "equilibrium" Gaussian distributions).

In fig. 1, we compare $W_1(x_0)$ and $W^{MC}(x_0)$ for $g=0.4$ and inverse temperatures varying from $\beta=0$ to $\beta=20$. Up to $\beta=8$ the agreement is excellent. From then on, $W_1(x_0)$ lies always higher than $W(x_0)$ in accordance with the bound (14). In fig. 2 we study the finite-L effect for $g=0.4$ and $\beta=20$. The dashed curve for $L=2$ is found by direct numerical integration of (19). We see that at such low temperatures the approximation fails in the central region while being surprisingly accurate at the boundary, in particular, the outer minima are well reproduced, as long as the size of L is so small that they are pronounced.

It will be interesting to study the properties of $W_1(x_0)$ in quantum field theories of finite-size systems.

References

[1] R.P. Feynman and H. Kleinert, Phys. Rev. A34 (1986) 5080.
[2] H. Kleinert, Phys. Letters A118 (1986) 267; W. Janke and H. Kleinert, Phys. Letters A118 (1986) 371;
R.D. Coalson, D.L. Freeman and J.D. Doll, J. Chem. Phys. 85 (1986) 4567.
[3] H. Kleinert, Phys. Letters A118 (1986) 195; Phys. Letters B181 (1986) 324.