EFECTIVE POTENTIALS FROM EFFECTIVE CLASSICAL POTENTIALS

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The effective potential (=Legendre transform of the generating functional) of a double-well potential is calculated via the recently proposed method of *effective classical potentials* (=potential $W(x_0)$ whose Boltzmann factor $\exp[-\beta W(x_0)]$ gives the distribution of path averages $x_0=[\int_0^\beta d\tau\, x(\tau)]/\beta$). The result is automatically convex and, down to very low temperatures, in excellent agreement with what is obtained by solving numerically the Schrödinger equation.

Recently, it has been pointed out that a quantity called the *effective classical potential* is useful in studying quantum mechanical systems at finite temperatures. If the partition function has the form

$$Z=\int \mathcal{D}x(\tau)\,\exp\left(-\int_0^\beta d\tau[\tfrac{1}{2}\dot{x}^2+V(x(\tau))]\right), \quad (1)$$

the effective classical potential $W(x_0)$ is defined by the path integral (1) at a fixed time average of the paths $x(\tau)$:

$$(1/\sqrt{2\pi\beta})\,\exp[-\beta W(x_0)]$$
$$\equiv\int \mathcal{D}x(\tau)\,\delta\left(x_0-\frac{1}{\beta}\int_0^\beta d\tau\, x(\tau)\right)$$
$$\times\exp\left(-\int_0^\beta d\tau[\tfrac{1}{2}\dot{x}^2+V(x(\tau))]\right). \quad (2)$$

In terms of $W(x_0)$, the partition function reduces to a single integral

$$Z=\int\frac{dx_0}{\sqrt{2\pi\beta}}\exp[-\beta W(x_0)], \quad (3)$$

which has the same form as the classical partition function

$$Z_{\rm cl}=\int\frac{dx_0}{\sqrt{2\pi\beta}}\exp[-\beta V(x_0)].$$

This is the reason for the above name for $W(x_0)$.

A simple extremal principle gives for $W(x_0)$ the following approximation [1]:

$$W(x_0)\approx W_1(x_0)$$
$$\equiv\frac{1}{\beta}\log\sh(\beta\Omega(x_0)/2)/[\beta\Omega(x_0)/2]$$
$$+V_{a^2}(x_0)-\tfrac{1}{2}\Omega^2(x_0)a^2(x_0), \quad (4)$$

where

$$a^2(x_0)\equiv[1/\beta\Omega^2(x_0)][\tfrac{1}{2}\beta\Omega(x_0)\,\cth\tfrac{1}{2}\beta\Omega(x_0)-1], \quad (5)$$

$$V_{a^2}(x_0)\equiv\int\frac{dx}{\sqrt{2\pi a^2}}\exp[-(1/2a^2)(x-x_0)^2]$$
$$\times V(x), \quad (6)$$

and

$$\Omega^2(x_0)\equiv\partial^2 V_{a^2}(x_0)/\partial x_0^2$$
$$=2\partial V_{a^2}(x_0)/\partial a^2. \quad (7)$$

For the anharmonic oscillator and the double-well potential, this approximation gave exellent free energies down to zero temperatures [1]. The mistake was nowhere larger than a few percent. Also particle distributions were found in reasonable agreement with

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the exact ones [2,3]. In this note we would like to use the same approximation to calculate the standard effective potential $V_{\rm eff}$ of quantum field theory. Recall that $V_{\rm eff}(X)$ is defined via the generating functional

$$Z[j] = \exp\{W[j]\}$$

$$= \int \mathcal{D}x \exp\left(- \int_0^\beta d\tau [\tfrac{1}{2}\dot{x}^2 + V(x(\tau)) - jx] \right). \quad (8)$$

The exponent $W[j]$ generates all connected Green's functions. The derivative

$$\delta W[j]/\delta j \equiv X[j] = X \equiv \langle x \rangle \quad (9)$$

is the response of the system to the external source $j(\tau)$. In analogy with magnetic systems, the function $X[j]$ will be referred to as *magnetization curve.*

The effective potential is given by the Legendre transform

$$\beta V_{\rm eff}(X) = - W[j] + \int d\tau\, Xj \quad (10)$$

evaluated at a *constant* external source j. Its derivative

$$\beta \partial V_{\rm eff}(X)/\partial X \equiv j(X) = j \quad (11)$$

is the inverse of the functional (6) evaluated at constant j.

Thus, if we succeed in finding the magnetization curve $X[j]$ for constant j, we can invert this function and integrate it to obtain $V_{\rm eff}(X)$, up to an irrelevant constant of integration. The effective potential is always a convex function of X. It is an old problem in quantum field theory that perturbative approaches to quantum systems with a non-convex potential $V(x)$, such as the double-well potential $V(x) = -\frac{1}{2}x^2 + \frac{1}{4}g\,x^4$, always fail to give a convex $V(x)$. Our approach has no problems in reaching this goal. The generating functional $W[j]$ at constant j, is simply given by

$$Z[j] = \exp\{W[j]\}$$

$$= \int \frac{dx_0}{\sqrt{2\pi\beta}} \exp\{-\beta[W(x_0) - jx_0]\}, \quad (12)$$

and

$$X[j] = Z^{-1}[j]$$

$$\times \int \frac{dx_0}{\sqrt{2\pi\beta}}\, x_0 \exp\{-\beta[W(x_0) - jx_0]\} \quad (13)$$

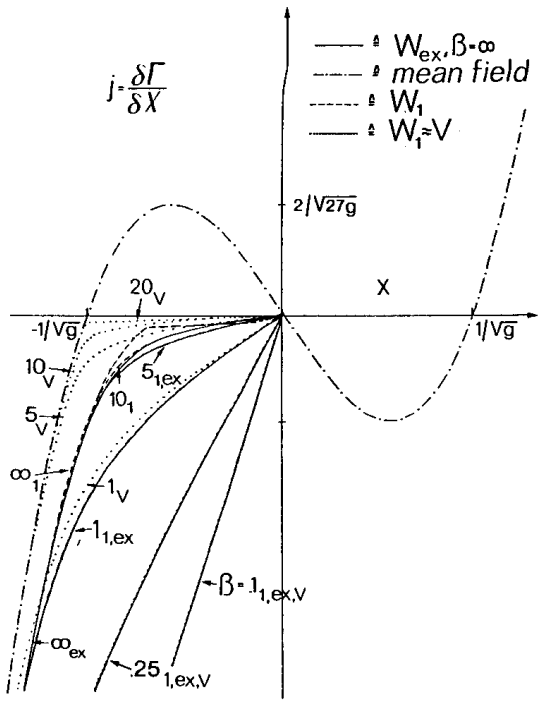

Fig. 1. The response curve $X = \langle x \rangle = X[j]$ for various constant sources j calculated once from our approximation to the effective classical potential $W(x_0) \approx W_1(x_0)$ (- - -) and once from the crude approximation $W(x_0) \approx V(x_0)$ (...). For $\beta \lesssim 0.1$, these agree with each other and with the exact curves (——) obtained by solving numerically the Schrödinger equation in an external field j. Our approximation $W_1(x_0)$ gives excellent agreement up to $\beta \approx 10$, which is quite a low temperature ($T \approx 1/10$).

has necessarily a positive derivative $\partial X/\partial j$ such that $\partial^2 V_{\rm eff}(X)/\partial X^2$ is positive and $V_{\rm eff}$ convex.

In fig. 1 we have plotted the magnetization curve (13) for $g = 0.4$ at various temperatures. For $\beta \gtrsim 10$, the exact magnetization curves (found by solving the lowest 8 eigenvalues of the Schrödinger equation for various j's) have practically reached the zero-temperature limit. We see that up to $\beta \approx 10$ our curves are in excellent agreement with the exact ones. In the opposite limit, for $\beta \lesssim 0.1$, the effective classical potential $W_1(X_0)$ becomes practically indistinguishable from the potential $V(x_0)$. This is seen by comparing our curves with those obtained by crudely approximating $W_1(x_0) \approx V(x_0)$ in eq. (13).

If the inverse temperature β is increased much further than $\beta \approx 10$, our approximation deteriorates. The reason for this can be seen in fig. 2, which shows the effective classical potential $W_1(x_0)$ for $g = 0.4$. For $\beta < 10$, it has two minima, and up to this point the

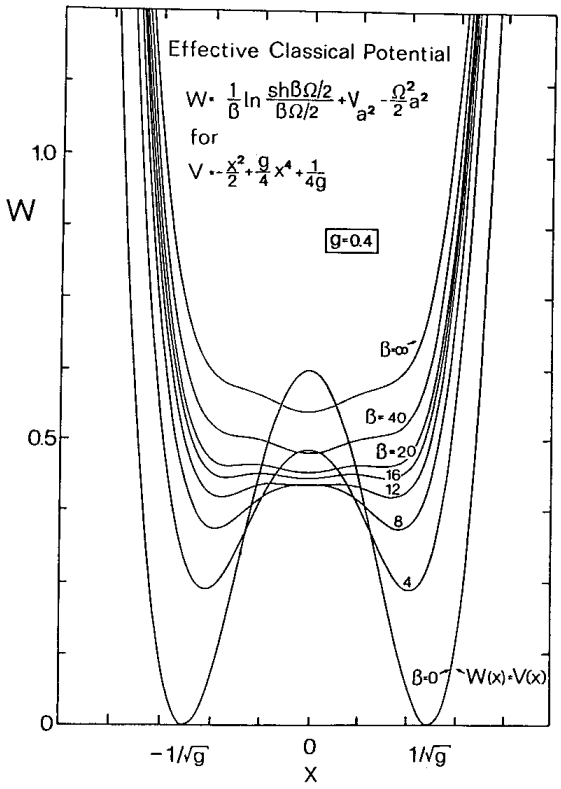

Fig.2. Our approximation $W_1(x_0)$ to the effective classical partition function $W(x_0)$ for the double-well potential $V(x_0) = -\frac{1}{2}x_0^2 + \frac{1}{4}gx_0^4$ at various temperatures. Up to $\beta \approx 10$, the approximation is excellent as witnessed by the agreement between exact and approximate magnetization curves in fig. 1 and the particle distributions shown in ref. [2].

magnetization curve is quite reliable. For large $\beta \gg 10$, however, the two minima flow together and the original double-well in $V(x_0)$ disappears completely. The single minimum at the origin reflects the fact that the zero-temperature limit of the free energy is equal to the expectation value of the hamiltonian in a single gaussian wave packet and that for $g=0.4$ this packet has to be situated at the origin. This is why the approximation becomes eventually bad. A superposition of two gaussians would really be needed. Thus the approximation can be used only up to $\beta \sim 10$, i.e. down to $T \gtrsim 1/10$.

It goes without saying that the approximation is superb for the anharmonic oscillator with positive curvature at the origin, for all g and β, down to zero temperature.

The method is sufficiently promising to warrant an application to field theories.

References

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