PARTICLE DISTRIBUTION FROM EFFECTIVE CLASSICAL POTENTIAL

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Received 17 June 1986; accepted for publication 1 September 1986

We show that the method of effective classical partition functions can be extended to find an approximation to the temperature dependent particle distributions of quantum systems which are quite accurate, even at low temperature.

Recently [1], an efficient method has been developed to replace the partition function of a quantum system at inverse temperature $\beta = 1/T$

$$Z \equiv \mathrm{e}^{-\beta F} \equiv \int \mathscr{D}x \exp\left(-\int_0^\beta \mathrm{d}\tau \, [\tfrac{1}{2}\dot{x}^2 + V(x)]\right) \tag{1}$$

by an approximate effective classical partition function

$$Z_1 = \mathrm{e}^{-\beta F_1} \equiv \int \frac{\mathrm{d}x_0}{\sqrt{2\pi\beta}} \exp[-\beta W_1(x_0)] \,, \tag{2}$$

which approaches Z very closely from below (i.e. $F_1 \geqslant F$), even at zero temperature. The approximate effective classical potential $W_1(x_0)$ is calculated from $V(x)$ by the following rules:

(1) Form the smeared-out potential

$$V_{a^2(x)}(x) \equiv \int_{-\infty}^{\infty} \frac{\mathrm{d}x'}{\sqrt{2\pi a^2}} \exp\left(-\frac{(x-x')^2}{2a^2}\right) V(x') \,, \tag{3}$$

with

$$a^2(x_0) \equiv \frac{2}{\beta} \sum_{n=1}^{\infty} \frac{1}{(2\pi n/\beta)^2 + \Omega^2(x_0)} \equiv \frac{[\beta\Omega(x_0)/2] \operatorname{cth}[\beta\Omega(x_0)/2] - 1}{\beta\Omega^2(x_1)} \,, \tag{4}$$

where $\Omega^2(x_0)$ is a variational parameter.

(2) Form

$$W_1(x_0) \equiv \beta^{-1} \log\left(\frac{\operatorname{sh}[\beta\Omega(x_0)/2]}{\beta\Omega(x_0)/2}\right) + V_{a^2(x_0)} - \tfrac{1}{2}\Omega^2(x_0) a^2(x_0) \,. \tag{5}$$

(3) Determine $\Omega^2(x_0)$ by minimizing $W_1(x_0)$, which gives

$$\Omega^2(x_0) = \partial^2 V_{a^2}(x_0)/\partial x_0^2 = 2\partial V_{a^2}(x_0)/\partial a^2 \,. \tag{6}$$

This result was derived by starting out from a trial partition function

[1] Supported in part by Deutsche Forschungsgemeinschaft under grant no. Kl 256.

$$Z_1 = \int \mathcal{D}x \exp\left(- \int_0^\beta \mathrm{d}\tau \, \{\tfrac{1}{2}\dot{x}^2(\tau) + \tfrac{1}{2}\Omega^2(x_0)[x(\tau) - x_0]^2\} \right) \mathrm{e}^{-\beta L_1(x_0)} , \tag{7}$$

where $x_0 = \beta^{-1} \int_0^\beta \mathrm{d}\tau \, x(\tau)$ is the time average of the path $x(\tau)$. By expanding $x(\tau)$ into its Fourier components

$$x(\tau) = x_0 + \sum_{n=1}^{\infty} (x_n \mathrm{e}^{\mathrm{i}\omega_n \tau} + \text{c.c.}) ,$$

with Matsubara frequencies $\omega_n = 2\pi n/\beta$, and using the measure

$$\int \mathcal{D}x = \int \frac{\mathrm{d}x_0}{\sqrt{2\pi\beta}} \prod_{n=1}^{\infty} \int \frac{\mathrm{d}x_n^{\mathrm{re}} \, \mathrm{d}x_n^{\mathrm{im}}}{\pi/\beta\omega_n^2} , \tag{8}$$

we integrated out all $n > 0$ components in Z_1 and found

$$Z_1 = \int \frac{\mathrm{d}x_0}{\sqrt{2\pi\beta}} \frac{\beta\Omega(x_0)/2}{\mathrm{sh}[\beta\Omega(x_0)/2]} \mathrm{e}^{-\beta L_1(x_0)} . \tag{9}$$

Then we determined $L_1(x_0)$ using Peierl's inequality:

$$Z \geqslant Z_1 \exp\left(\int_0^\beta \mathrm{d}\tau \, \langle \{ V(x(\tau)) - \tfrac{1}{2}\Omega^2(x_0)[x(\tau) - x_0]^2 - L_1(x_0) \} \rangle_1 \right) , \tag{10}$$

where $\langle \ \rangle_1$ is the expectation with respect to the integrand of the partition function Z. This gave

$$L_1(x_0) = V_{a^2(x_0)}(x_0) - \tfrac{1}{2}\Omega^2(x_0) a^2(x_0) , \tag{11}$$

with $a^2(x_0)$ of eq. (5), which amounts to the above stated rules.

In ref. [1] we have applied this method to the potentials $V(x) = \pm\frac{1}{2}x^2 + \frac{1}{4}gx^4$ and shown that, even for very strong anharmonicity, the approximate free energy F_1 differs from the exact F by at most a few percent, down to zero temperature. The reason is that F_1 at zero temperature tends to the expectation value of the energy in an optimal gaussian wavefunction and this is known to be a reasonable approximation to the true ground state energy whenever the potential is smoothly curved around its minimum.

The purpose of this note is to extend the method in such a way that it gives us an approximation also to the particle distribution functions of quantum systems

$$\rho(x_a) = Z^{-1}(x_a \, \beta \,|\, x_a \, 0) = Z^{-1} \int_{x(0) = x(\beta) = x_a} \mathcal{D}x \exp\left(- \int_0^\beta \mathrm{d}\tau \, [\tfrac{1}{2}\dot{x}^2 + V(x)] \right) , \tag{12}$$

where x_a is the initial = final position of the particle's periodic paths. The approximation to $\rho(x_a)$ is provided by the particle density $\rho_1(x_a)$ associated with the trial partition function Z_1. In order to obtain it we insert into the path integral for Z_1 a δ-function enforcing that $x_a = x(0) = x_0 + \sum_{n=1}^{\infty} (x_n + \text{c.c.})$ and have

$$\rho_1(x_a) = Z_1^{-1} \int \mathcal{D}x \exp\left(- \int_0^\beta \mathrm{d}\tau \, \{\tfrac{1}{2}\dot{x}^2 + \tfrac{1}{2}\Omega^2(x_0)[x(\tau) - x_0]^2\} \right) \mathrm{e}^{-\beta L_1(x_0)}$$
$$\times \int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda}{2\pi} \exp\left[\mathrm{i}\lambda \left(x_a - x_0 - \sum_{n=1}^{\infty} (x_n + \text{c.c.}) \right) \right] . \tag{13}$$

Performing now the x_n, $n > 0$, integrals yields

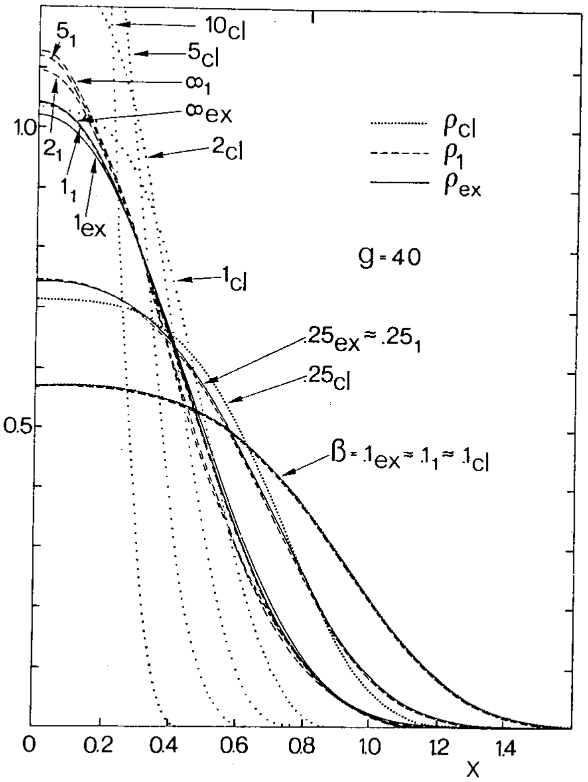

Fig. 1. The particle density $\rho_1(x_a)$ as compared with the exact density $\rho(x_a)$ (calculated from the Schrödinger wavefunctions) and the classical one $\rho_{cl}(x_a)$, for the anharmonic oscillator potential $V(x)=\frac{1}{2}x^2+\frac{1}{4}gx^4$ with $g=40$.

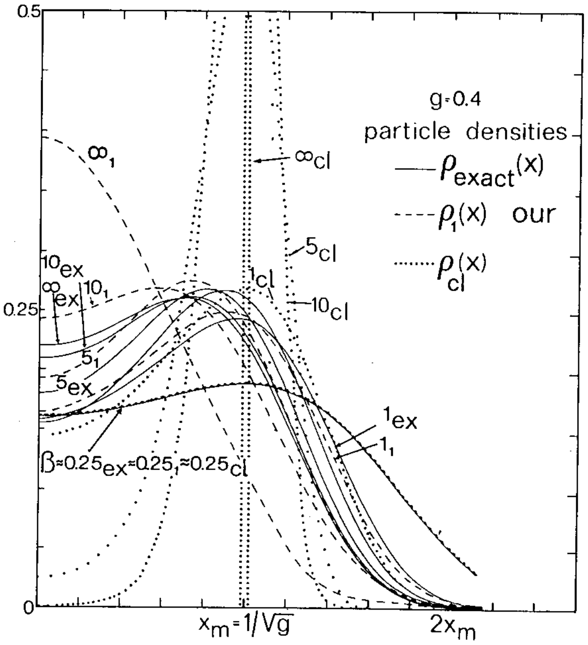

Fig. 2. The same plot as in fig. 1, but for the double-well potential $V(x)=-\frac{1}{2}x^2+\frac{1}{4}gx^4$ at the coupling strength $g=0.4$. Our approximation becomes bad for $\beta \gtrsim 5$ for reasons explained in the text.

$$\rho_1(x_a)=Z_1^{-1}\int \frac{dx_0}{\sqrt{2\pi\beta}}\,\frac{\beta\Omega(x_0)/2}{\mathrm{sh}[\beta\Omega(x_0)/2]}\,e^{-\beta L_1(x_0)}\int\frac{d\lambda}{2\pi}\exp\left[i\left(\lambda x_a - x_0-\sum_{n=1}^{\infty}(x_n+\text{c.c.})\right)\right]$$
$$=Z_1^{-1}\int_{-\infty}^{\infty}\frac{dx_0}{\sqrt{2\pi\beta}}\,\frac{\exp[-(x_a-x_0)^2/2a^2(x_0)]}{\sqrt{2\pi a^2(x_0)}}\,e^{-\beta W_1(x_0)}\,. \tag{14}$$

This is a super-position of gaussians of varying widths with the distribution given by the effective classical Boltzmann factor $e^{-\beta W_1(x_0)}$. It has the proper normalization $\int_{-\infty}^{\infty} dx_a\,\rho_1(x_a)=1$. At high temperatures, $a^2\to\frac{1}{12}\beta\to 0$, $W_1(x)\to V(x)$, and $\rho_1(x_a)$ tends to the classical limit

$$\rho_1(x_a)\xrightarrow[\beta\to 0]{}\rho_{cl}(x_a)\equiv Z_{cl}^{-1}e^{-\beta V(x_a)}\,. \tag{15}$$

At low temperatures, the gaussians cluster mostly around the minima of $W_1(x_0)$.

A comparison with the exact distribution $\rho(x_a)$ of the anharmonic oscillator and the double-well potential is shown in figs. 1 and 2, respectively, for two representative coupling strengths. At high temperatures, the agreement is excellent for all g. At low temperatures, the distribution of the anharmonic oscillator is slightly exaggerated at the origin, since the approximation $W_1(x_0)$ squeezes an optimal gaussian wave packet into the potential $V(x)=\frac{1}{2}x^2+\frac{1}{4}gx^4$. For the double-well potential, the agreement is worst if g lies near $g=0.4$. The deterioration sets in at around $\beta\gtrsim 5$ (see fig. 2) due to the eventual centering of the optimal gaussian wave packets in eq.

(20) at the origin (compare fig. 3 of ref. [1]). For large g, this is acceptable and the agreement is much better than for $g=0.4$. For very small $g \ll 0.4$, when the central barrier is very high, the agreement is again very good since there the optimal gaussians accumulate at the two minima $\pm x_{\text{min}} \neq 0$ and reproduces the proper double peak in the particle distribution at low temperature.

Reference

[1] H. Kleinert and R.P. Feynman, to be published.