EFFECTIVE CLASSICAL POTENTIAL AND PARTICLE DISTRIBUTION OF A COULOMB SYSTEM

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As a further test of the quality of the recently proposed method of effective classical potentials, we calculate the distribution function of a particle in a Coulomb field and compare the result with the exact distribution.

Recently, a new approximation has been proposed to calculate the partition function of a quantum mechanical system [1]. It is based on the Fourier decomposition of the path integral at finite temperature $T\equiv 1/\beta$

$$Z\equiv e^{-\beta F}\equiv \int \mathscr{D}^3x \exp\left(-\int_0^\beta d\tau\,[\tfrac{1}{2}\dot{\boldsymbol{x}}^2+V(\boldsymbol{x}(\tau))]\right)$$

$$=\int \frac{d^3x_0}{(2\pi\beta)^{3/2}}\prod_{n=1}^{\infty}\int\frac{d^3x_n^{\rm re}d^3x_n^{\rm im}}{[\pi/(\beta\omega_n^2)]^3}\exp\left[-\beta\sum_{n=1}^{\infty}\omega_n^2\boldsymbol{x}_n^2-\int_0^\beta d\tau\, V\left(\boldsymbol{x}_0+\left(\sum_{n=1}^{\infty}e^{-i\omega_n\tau}\boldsymbol{x}_n+\text{c.c.}\right)\right)\right]. \tag{1}$$

Since $\omega_n=(2\pi/\beta)n$, the $\boldsymbol{x}_n^{\rm re}, \boldsymbol{x}_n^{\rm im}$ integrations for $n>0$ are rapidly convergent and can be treated in a self-consistent one-loop approximation, leaving only the x_0 integral to be done with more care. The result is an approximation to the effective classical potential $W(\boldsymbol{x}_0)$, defined by

$$Z\equiv\int\frac{d^3x_0}{(2\pi\beta)^{3/2}}e^{-\beta W(\boldsymbol{x}_0)}, \tag{2}$$

which is given by

$$W(\boldsymbol{x}_0)\approx W_1(\boldsymbol{x}_0)=\frac{3}{\beta}\log\left(\frac{\text{sh}[\beta\Omega(\boldsymbol{x}_0)/2]}{\beta\Omega(\boldsymbol{x}_0)/2}\right)+V_{a^2(\boldsymbol{x}_0)}(\boldsymbol{x}_0)-\tfrac{3}{2}\Omega^2(\boldsymbol{x}_0)a^2(\boldsymbol{x}_0), \tag{3}$$

where

$$V_{a^2}(\boldsymbol{x}_0)=\int\frac{d^3x}{(2\pi a^2)^{3/2}}\exp\left(-\frac{(\boldsymbol{x}-\boldsymbol{x}_0)^2}{2a^2}\right)V(\boldsymbol{x}) \tag{4}$$

is a potential smeared out with a gaussian of width a^2. The corresponding partition function Z_1 approximates Z from below. The optimal $W_1(\boldsymbol{x}_0)$ is reached for

$$a^2(\boldsymbol{x}_0)=[\beta\Omega^2(\boldsymbol{x}_0)]^{-1}\{[\beta\Omega(\boldsymbol{x}_0)/2]\,\text{cth}[\beta\Omega(\boldsymbol{x}_0)/2]-1\}, \tag{5}$$

where the frequency $\Omega(\boldsymbol{x}_0)$ is determined self-consistently from the equation

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$$\Omega^2(\boldsymbol{x}_0) = \tfrac{2}{3}(\partial/\partial a^2) V_{a^2}(\boldsymbol{x}_0) = \tfrac{1}{3}(\partial/\partial \boldsymbol{x}_0)^2 V_{a^2}(\boldsymbol{x}_0) . \tag{6}$$

For a one-dimensional oscillator [1] and a double-well potential [2], the free energy calculated from Z_1, $F_1 \equiv -\beta^{-1}\log Z_1$, was shown to reproduce the exact free energy F to within a few percent, even at zero temperature. The accuracy is explained by the fact that the zero-temperature limit of F_1 coincides with the optimal expectation value of the hamiltonian operator in a gaussian wave packet, which is known to be a good approximation to the ground state energy for many smooth potentials.

For a Coulomb system with a hamiltonian

$$\hat{H} = -\tfrac{1}{2}\partial^2 - 1/r \tag{7}$$

the potential is not smooth. Nevertheless, the smeared out potential can easily be calculated to be

$$V_{a^2}(r_0) = -\frac{1}{r_0}\frac{2}{\sqrt{\pi}} \int_0^{r_0/\sqrt{2a^2}} \mathrm{d}\xi\, \mathrm{e}^{-\xi^2} = -\frac{1}{r_0}\,\mathrm{erf}(r_0/\sqrt{2a^2}) . \tag{8}$$

Hence

$$\Omega^2(r_0) = \frac{2}{3}\frac{1}{\sqrt{2\pi}}\frac{1}{(a^2)^{3/2}}\,\mathrm{e}^{-r_0^2/2a^2} . \tag{9}$$

The optimal expectation of a gaussian wave packet

$$\psi(\boldsymbol{x}) = (2\pi a^2)^{-3/4}\,\mathrm{e}^{-\boldsymbol{x}^2/4a^2} \tag{10}$$

becomes

$$E^0 \equiv \min\{3/8a^2 + V_{a^2}(0)\} = -3/8a^2_{\min} = -4/3\pi \approx -0.4244 , \tag{11}$$

with the minimum lying at $a^2_{\min} = 9\pi/32$. The value -0.4244 is only 15% smaller than the true ground state energy $-1/2$ such that $W_1(r_0)$ should be a reasonable approximation to the effective classical potential also in this case.

It is the purpose of this note to calculate the particle distribution of the Coulomb system which can be approximated by the same method. It is given by [2]

$$\rho(\boldsymbol{x}) \approx \rho_1(\boldsymbol{x}) = \int \frac{\mathrm{d}^3 x_0}{[2\pi a^2(r_0)]^{3/2}} \exp\left(-\frac{(\boldsymbol{x}-\boldsymbol{x}_0)^2}{2a^2(\boldsymbol{x}_0)}\right) \frac{\exp[-\beta W_1(\boldsymbol{x}_0)]}{(2\pi\beta)^{3/2}}$$
$$= \frac{1}{r}\int_0^\infty \frac{\mathrm{d}r_0\, r_0}{\sqrt{2\pi a^2(r_0)}}\left[\exp\left(-\frac{(r-r_0)^2}{2a^2(r_0)}\right) - \exp\left(-\frac{(r+r_0)^2}{2a^2(r_0)}\right)\right]\frac{\exp[-\beta W_1(r_0)]}{(2\pi\beta)^{3/2}} , \tag{12}$$

where $a^2(r_0)$, $\Omega^2(r_0)$ are found by iterating at each r_0 eqs. (5) and (6).

In fig. 1 we have plotted $W_1(r_0)$ for various temperatures. The $1/r$ singularity is smoothed out by quantum fluctuations. For $T \to 0$, the minimum of $W_1(r_0)$ is given by E^0 of eq. (8) and for $T \to \infty$, $W_1(r_0)$ approaches the classical potential $V(r_0) = -1/r_0$. In order to compare with an earlier calculation of the densities [3], the temperatures are given in K. The connection with our natural units, in which $m \equiv m_e m_p/(m_e + m_p) = e^2 = \hbar = 1$, is

$$\beta = (1/k_B T) e^4 m/\hbar^2 = 315\,605.22\ \mathrm{K}/T . \tag{13}$$

Fig. 2 shows the distribution itself, except for a factor $(2\pi\beta)^{3/2}$ i.e.,

$$g_2(\boldsymbol{x}) \equiv (2\pi\beta)^{3/2}\rho(\boldsymbol{x}) \tag{14}$$

in order to have a simple high-temperature limit

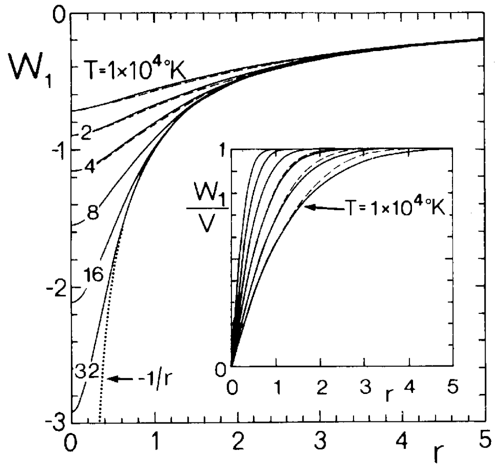

Fig. 1. The approximate effective potential $W_1(r_0)$ for various temperatures, once in the isotropic and once in the anisotropic approximation (explained in the text). The improvement is better visible in the insert where we have plotted W_1/V. The corresponding reduced inverse temperatures $\beta=1/T$ are 31.56, 15.78, 7.89, 3.945, 1.9725, 0.9863, 0, respectively.

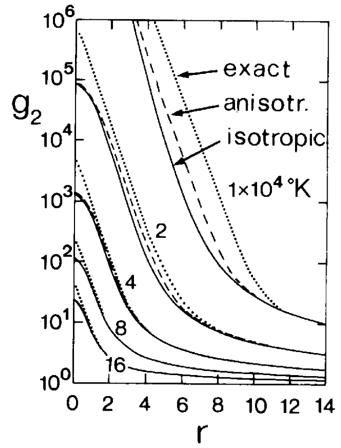

Fig. 2. The particle distribution $g_2(\boldsymbol{x})\equiv(2\pi\beta)^{3/2}\rho(\boldsymbol{x})$ for the same temperatures as in fig. 1, once in the isotropic and once in the anisotropic approximation (explained in the text). Comparison is made with the exact distributions as given in ref. [3]. For low and intermediate temperatures, it is sufficient to use the states of the lowest three energy levels and the quantum mechanical expression $\rho(\boldsymbol{x})=\pi^{-1}e^{-2r}e^{\beta/2}+(1/8\pi)(1-r+r^2/2)e^{-r}e^{\beta/8}+(1/3^8\pi)(243-324r+216r^2-48r^3+4r^4)e^{-2r/3}e^{\beta/18}$.

$$\log g_2(\boldsymbol{x})/\beta \xrightarrow[T\to\infty]{} 1/r\,.$$

The agreement with the exact distributions is becoming unsatisfactory at $T\lesssim 2\times10^4$ K. This corresponds to $\beta>15$ which is quite a low temperature, on the natural energy scale. The approximation is therefore astonishingly reliable.

The intermediate r regime can be improved by using the anisotropic version of the same procedure. For this one takes a smear-out parameter which is different for radial and azimuthal directions and calculates

$$V_{a_L^2,a_T^2}(r_0)=-\int\frac{dz}{\sqrt{2\pi a_L^2}}\int\frac{dx\,dy}{2\pi a_T^2}\exp\left(-\frac{(z-r_0)^2}{2a_L^2}-\frac{x^2+y^2}{2a_T^2}\right)\frac{1}{r}$$
$$=-\sqrt{a_L^2/2\pi}\int_{-1}^{1}d\lambda\,\frac{\exp[-(r_0^2/2a_L^2)\lambda^2]}{a_L^2(1-\lambda^2)+a_T^2\lambda^2}\,. \qquad (15)$$

From this one finds

$$\Omega_T^2(r_0)\equiv\frac{\partial}{\partial a_T^2}V_{a_T^2,a_L^2}=\sqrt{a_L^2/2\pi}\int_{-1}^{1}d\lambda\,\frac{\lambda^2\exp[-(r_0^2/2a_L^2)\lambda^2]}{[a_L^2(1-\lambda^2)+a_T^2\lambda^2]}\,,$$

$$\Omega^2(r_0)\equiv\tfrac{1}{3}[\Omega_L^2+2\Omega_T^2]=\tfrac{1}{3}[\partial/\partial a_L^2+\partial/\partial a_T^2]\,V_{a_T^2,a_L^2}=\frac{2}{3}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{a_L^2a_T^4}}\exp(-r_0^2/2a_L^2)\,, \qquad (16)$$

where

$$a_{L,T}^2=(1/\beta\Omega_{L,T}^2)[(\beta\Omega_{L,T}/2)\,\mathrm{cth}(\beta\Omega_{L,T}/2)-1]\,. \qquad (17)$$

The iterative solution of these equations yields the approximation to the effective classical potential

$$W(r_0) \approx W_1^{\text{anis}}(r_0) = \frac{1}{\beta}\left(\log \frac{\text{sh}[\beta\Omega_L(r_0)/2]}{\beta\Omega_L(r_0)/2} + 2\log \frac{\text{sh}[\beta\Omega_T(r_0)/2]}{\beta\Omega_T(r_0)/2} \right)$$

$$+ V_{a_L^2, a_T^2(r_0)}(r_0) - \tfrac{1}{2}[\Omega_L^2(r_0)a_L^2(r_0) + 2\Omega_T^2(r_0)a_T^2(r_0)] \,. \quad (18)$$

Fig. 1 shows the comparison with the isotropic case. The associated density

$$\rho(r) \approx \rho_1^{\text{anis}}(r) = \int d^3x_0 \left(\frac{\exp[-(z_0 - r)^2/2a_L^2]}{\sqrt{2\pi a_L^2(r_0)}} \frac{\exp(-x_0^2/2a_T^2)}{2\pi a_T^2(r_0)} \frac{\exp[-\beta W_1(r_0)]}{(2\pi\beta)^{3/2}} \right)$$

$$= 2\pi \int_0^\infty dr_0 \int_{-1}^{1} d\lambda \frac{\exp[-(\lambda r_0 - r)^2/2a_L^2]}{\sqrt{2\pi a_L^2(r_0)}} \frac{\exp[-r_0^2(1-\lambda^2)/2a_T^2]}{2\pi a_T^2(r_0)} \frac{\exp[-\beta W_1(r_0)]}{(2\pi\beta)^{3/2}} \quad (19)$$

is plotted in fig. 2 (after removing the factor $(2\pi\beta)^{-3/2}$). We observe that, for low temperatures, the intermediate r regime is markedly improved with respect to the isotropic calculation.

In conclusion we see that as long as the smeared out potential $V_{a^2}(r_0)$ exists, the method may be of practical use also in systems whose potential is not smooth.

References

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