E0070: Ergodic density

Submitted by: Alexander Elikashvili

The problem:

Assuming a microcanonical ensemble with energy E find an expression for probability density $\rho(x)$ of a particle which is confined by a potential $V(x)$. Distinguish between 1, 2 and 3 dimensional cases. In particular show that in 2D case the probability density forms a step function. Contrast your results with the canonical expression $\rho(x) \propto \exp(-\beta V(x))$.

The solution:

$$\rho(x) = \frac{1}{(2\pi)^D} \int \rho(x,p)\delta(H(x,p) - E)d^D p$$

where D stands for dimension number and $\rho(x,p) = \frac{1}{g_D(E)}$, $g_D(E) = \frac{1}{(2\pi)^D} \iint \delta(H(x,p) - E)d^D x d^D p$. Following mathematical relations will be helpful for solving the problem:

$$(1) \quad \delta(f(x)) = \sum_i \frac{\delta(x - x_i)}{|f'(x_i)|}, \quad f(x_i) = 0 \qquad\qquad (2) \quad \Theta(x) = \begin{cases} 0, & x < 0 \\ 1, & x \geq 0 \end{cases}$$

1D case:

$$\rho(x) = \frac{1}{2\pi g_1(E)} \int \delta\left(\frac{p^2}{2m} + V(x) - E\right) dp$$

One can distinguish between two possible solutions:

($*$) First case is when $V(x) - E > 0$:

$$\rho(x) = \frac{1}{2\pi g_1(E)} \int \delta\left(\frac{p^2}{2m} + V(x) - E\right) dp = 0$$

($**$) Second case is when $V(x) - E < 0$, so with the help of relation (1) one gets:

$$\rho(x) = \frac{1}{2\pi g_1(E)} \int_{-\infty}^{\infty} \left(\frac{\delta\left(p - \sqrt{2m(E - V(x))}\right)}{|\frac{p}{m}|} + \frac{\delta\left(p + \sqrt{2m(E - V(x))}\right)}{|\frac{p}{m}|} \right) dp = \frac{1}{2\pi g_1(E)} \sqrt{\frac{2m}{E - V(x)}}$$

Using relation (2) one can combine solution ($*$) with ($**$) and write:

$$\rho(x) = \frac{1}{2\pi g_1(E)} \sqrt{\frac{2m}{E - V(x)}} \Theta(E - V(x)) \qquad g_1(E) = \frac{1}{2\pi} \int \sqrt{\frac{2m}{E - V(x)}} \Theta(E - V(x))\, dx$$

2D case:

$$\rho(\vec{r}) = \frac{1}{(2\pi)^2 g_2(E)} \int \delta\left(\frac{\vec{p}^2}{2m} + V(\vec{r}) - E\right) dp_x dp_y$$

Just like in 1D case one has two possible solutions:

($*$) First one is when $V(\vec{r}) - E > 0$.

$$\rho(\vec{r}) = \frac{1}{(2\pi)^2 g_2(E)} \iint \delta\left(\frac{\vec{p}^2}{2m} + V(\vec{r}) - E\right) dp_x dp_y = 0$$

($**$) Second case is when $V(\vec{r}) - E < 0$, so with the help of relation (1) one gets:

$$\rho(\vec{r}) = \frac{1}{2\pi g_2(E)} \int_0^\infty \left(\frac{\delta\left(p - \sqrt{2m\left(E - V\left(\vec{r}\right)\right)}\right)}{|\frac{p}{m}|} + \frac{\delta\left(p + \sqrt{2m\left(E - V\left(\vec{r}\right)\right)}\right)}{|\frac{p}{m}|} \right) p dp = \frac{m}{2\pi g_2(E)}$$

Using relation (2) one can combine solution ($*$) with ($**$) and write:

$$\rho(\vec{r}) = \frac{m}{2\pi g_2(E)} \Theta\left(E - V\left(\vec{r}\right)\right) \qquad g_2(E) = \frac{m}{2\pi} \iint \Theta(E - V(\vec{r})) dx dy$$

3D case:

$$\rho(\vec{r}) = \frac{1}{(2\pi)^3 g_3(E)} \int \delta\left(\frac{\vec{p}^2}{2m} + V(\vec{r}) - E\right) dp_x dp_y dp_z$$

In complete analogy with 1D and 2D cases one has two possible solutions:

($*$) First one is when $V(\vec{r}) - E > 0$.

$$\rho(\vec{r}) = \frac{1}{(2\pi)^3 g_3(E)} \iiint \delta\left(\frac{\vec{p}^2}{2m} + V(\vec{r}) - E\right) dp_x dp_y dp_z = 0$$

($**$) Second case is when $V(\vec{r}) - E < 0$, so with the help of relation (1) one gets:

$$\rho(\vec{r}) = \frac{1}{2\pi^2 g_3(E)} \int_0^\infty \left(\frac{\delta\left(p - \sqrt{2m\left(E - V\left(\vec{r}\right)\right)}\right)}{|\frac{p}{m}|} + \frac{\delta\left(p + \sqrt{2m\left(E - V\left(\vec{r}\right)\right)}\right)}{|\frac{p}{m}|} \right) p^2 dp = \frac{m\sqrt{2m\left(E - V(\vec{r})\right)}}{2\pi^2 g_3(E)}$$

Using relation (2) one can combine solution ($*$) with ($**$) and write:

$$\rho(\vec{r}) = \frac{m\sqrt{2m\left(E - V(\vec{r})\right)}}{2\pi^2 g_3(E)} \Theta\left(E - V\left(\vec{r}\right)\right) \qquad g_3(E) = \iiint \frac{m\sqrt{2m\left(E - V(\vec{r})\right)}}{2\pi^2} \Theta\left(E - V\left(\vec{r}\right)\right) dx dy dz$$

In comparision with canonical ensemble microcanonical probability density has a wide range distribution, while canonical expression ρ is concentrated around the minimum of the confining potential V.