E0070: The ergodic density $\rho(x)$

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The problem:

Find an expression for $\rho(x)$ of a particle which is confined by a potential $V(x)$, assuming that the its state is microcannonical with energy E. Distinguish the special cases of $d = 1, 2, 3$ dimensions. In particular show that in the in the $d = 2$ case the density forms a step function. Contrast your results with the canonical expression $\rho(x) \propto exp(-\beta V(x))$.

The solution:

In the microcanonical ensemble with energy E the density $\rho(x)$ in d-dimensions is given by

$$\rho(x) = \frac{\int \frac{d^d p}{(2\pi)^d} \delta(H(x,p) - E)}{\int \frac{d^d x d^d p}{(2\pi)^d} \delta(H(x,p) - E)} \equiv \frac{\bar{\rho}_E(x)}{g(E)}, \tag{1}$$

where $g(E)$ is the density of states (DOS). We assume that $H(x,p) = \frac{p^2}{2m} + V(x)$, and that $V(x \to \pm\infty) = \infty$. Since H depends only on the magnitude of P, while evaluating $\bar{\rho}_E(x)$ in any dimension we make the integration over the momentum p in spherical coordinate. The constant which is the result of the angular constant is denoted by C_d, where $C_1 = 2$, $C_2 = 2\pi$, $C_3 = 4\pi$.

$$\bar{\rho}_E(x) = \int \frac{d^d p}{(2\pi)^d} \delta(H(x,p) - E) = C_d \int_0^\infty dp p^{d-1} \delta\left(\frac{p^2}{2m} - E + V(x)\right). \tag{2}$$

Now we use the fact that

$$\int_{-\infty}^{\infty} f(x)\, \delta(g(x))\, dx = \sum_i \frac{f(x_i)}{|g'(x_i)|}, \tag{3}$$

which implies

$$\begin{aligned} \bar{\rho}_E(x) &= C_d \frac{m}{\sqrt{2m(E - V(x))}} \int_0^\infty dp p^{d-1} \delta\left[p - \sqrt{2m(E - V(x))}\right] \\ &= C_d m \left[2m(E - V(x))\right]^{\frac{d}{2}-1} \Theta(E - V(x)), \end{aligned} \tag{4}$$

where $\Theta(x)$ is the step function. Accordingly

$$g(E) = \int d^d x \bar{\rho}_E(x) = C_d m \int_{V(x) \le E} d^d x \left[2m(E - V(x))\right]^{\frac{d}{2}-1} \equiv C_d m V_{d,E} \tag{5}$$

Substituting Eqs. (4) and (5) in Eq. (1), we get

$$\rho(x) = \frac{1}{V_{d,E}} \left[2m(E - V(x))\right]^{\frac{d}{2}-1} \Theta(E - V(x)) \tag{6}$$

Specifically

$$d = 1 : \rho(x) = \frac{\Theta(E - V(x))}{V_{1,E}\sqrt{2m(E - V(x))}} \tag{7}$$

$$d = 2 : \rho(x) = \frac{\Theta(E - V(x))}{V_{2,E}} \tag{8}$$

$$d = 3 : \rho(x) = \frac{\sqrt{2m(E - V(x))}\Theta(E - V(x))}{V_{3,E}}. \tag{9}$$

One can see that for $d = 2$ a step function is indeed received.

In the canonical ensemble $\rho(x) \sim e^{-\beta V(x)}$, which means that $\rho(x)$ is exponentially localized around the minimum of $V(x)$. In the microcanonical ensemble high energy may lead to larger phase space, and therefore to wider density distribution, while in the canonical ensemble the system is restricted to the ground states, thus concentrated around the minimum of the confining potential.