

Finding constraint minima for separable anharmonic potential with cubic anharmonicity

Let us find minimum of the function

$$W = \sum_{n=1}^N \frac{\alpha}{2} x_n^2 \quad (1)$$

under the restriction $H = E$ where

$$H = \sum_{n=1}^N \left(\frac{1}{2} x_n^2 + \frac{1}{6} f x_n^3 \right). \quad (2)$$

Since $\vec{\nabla} W = \lambda \vec{\nabla} H$ for some λ , then we have a system of identical equations $\alpha x_n = \lambda (x_n + \frac{1}{2} x_n^2)$ each of them with two roots, $x_n = 0$ or $x_n = \frac{2(\alpha - \lambda)}{f\lambda}$. If there are M nonzero roots, then

$$W = 2\alpha M \left(\frac{\alpha - \lambda}{f\lambda} \right)^2, \quad (3)$$

and

$$H = \frac{2M}{3f^2\lambda^3} (\alpha - \lambda)^2 (2\alpha + \lambda). \quad (4)$$

Using a relation $W = \frac{3\alpha\lambda}{2\alpha + \lambda} H$ that follows from (3) and (4) and a condition $H = E$, Eq. (3) is simplified as

$$W = \frac{3}{2\lambda^{-1} + \alpha^{-1}} E. \quad (5)$$

From (5), it follows that minimum of W is reached for minimum of possible λ . The parameter λ implicitly depends on M according to the formula

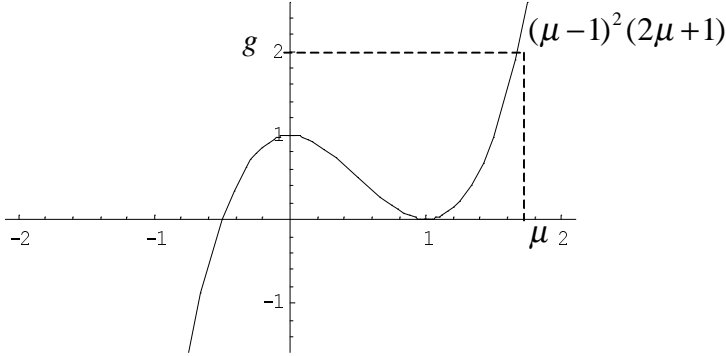
$$\frac{2M}{3f^2\lambda^3}(\alpha - \lambda)^2(2\alpha + \lambda) = E \quad (6)$$

that follows from (4) and the restriction $H = E$. So, the problem reduces to finding of minimum root λ of Eq. (6) for all possible $M = 0, 1, \dots, N$, the number of nonzero x_n .

Eq. (6) is simplified as

$$(\mu - 1)^2(2\mu + 1) = g, \quad (7)$$

where $\mu = \alpha / \lambda$ and $g = \frac{3Ef^2}{2M}$. Eq. (7) has only one parameter, g , and it is quite elementary to prove that its maximal root increases when g increases (for positive g), see the following figure.



So, λ is minimal when the root μ is maximal, or for a maximal possible g that is for $M = 1$.

Finally, we found that the minimum of W is attained at one of N equivalent points $(0, \dots, x_n, 0, \dots, 0)$ where $x_n = \frac{2(\alpha - \lambda)}{f\lambda}$, $\lambda = \alpha / \mu$ and μ is the maximal root of Eq. (6) with $M = 1$.

There is an explicit formula for this root of the cubic equation:

$$\mu = \frac{1}{2}(1 + D + D^{-1}), \quad (8)$$

where $D = \left[2g - 1 + 2(g^2 - g)^{1/2}\right]^{1/3}$, $g = \frac{3}{2}Ef^2$.