

Quartic potential calculation

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1 Goal

Figure out the relation between some of the important parameters for a double-well formed by quartic potential

2 Parameters

Focusing on the two wells, the intuitive parameters includes

1. Confinement for each well (the coefficient of x^2)
2. Well separation
3. Well height difference

The barrier height between the wells could be useful as well.

3 Setup

Let's say one of the well (let's say the left one) is located at $(0,0)$ and has the form $\frac{x^2}{2}$. The most generic quartic potential we can write is then

$$U = \frac{ax^4}{4} + \frac{bx^3}{3} + \frac{x^2}{2}$$

note that the trap centering at $(0,0)$ eliminates the linear and constant terms.

4 Derivation

Derivatives

$$\begin{aligned}U' &= ax^3 + bx^2 + x \\U'' &= 3ax^2 + 2bx + 1\end{aligned}$$

At the bottom of the well(s) (and the top of the barrier) we have

$$\begin{aligned}0 &= U' \\&= ax^3 + bx^2 + x \\&= (ax^2 + bx + 1)x\end{aligned}$$

Solution $x = 0$ is the one we fixed and for the other well and the barrier we have

$$ax^2 = -(bx + 1)$$

Assuming a real solution x exist

$$\begin{aligned} U'' &= 3ax^2 + 2bx + 1 \\ &= -3(bx + 1) + 2bx + 1 \\ &= -bx - 2 \\ U &= \frac{-(bx + 1)x^2}{4} + \frac{bx^3}{3} + \frac{x^2}{2} \\ &= -\frac{bx^3}{4} - \frac{x^2}{4} + \frac{bx^3}{3} + \frac{x^2}{2} \\ &= \frac{bx^3}{12} + \frac{x^2}{4} \\ &= \frac{x^2}{4} \left(1 + \frac{bx}{3} \right) \end{aligned}$$

We can pick the position of the second well x_2 and $\alpha \equiv -bx_2 - 2$ as the free parameters.

1. The confirmment for the second well, relative to the first well is α .
2. The well separation is simply x_2 .
3. The well height difference is $\frac{x_2^2(1 - \alpha)}{12}$

Note that this can describe both the second well and the barrier. The condition for this describing the well, instead of the barrier is simply $\alpha > 0$.

With a fixed ratio of the potential the well height difference goes down quadratically and the only way to get true zero well height differences is for $\alpha = 1$, which means symmetric well.