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 confirment 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 $\dfrac{x_2^2(1 - \alpha)}{12}$

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.

Converting back to the polynomial coefficients so that it's easy to tell what are parameters that makes sense

$$\begin{aligned}
b =& -\frac{\alpha + 2}{x_2}\\
a =& \frac{\alpha + 1}{x_2^2}
\end{aligned}$$

As $x_2 \to 0$, a diverges for $\alpha \neq -1$ and b diverges for $\alpha \neq -2$, so this description is not suitable when the two wells merges together. In the actual merging process for two wells in quartic potential, the quadratic term will disappear when the traps are merged together. During that process, the confinement of each of the wells will goes to zero and that cannot be covered by our model (it could be if we add another scaling factor and make it proportional to x_2^2).