

Errata: A dimer method for finding saddle points on high dimensional potential surfaces using only first derivatives

The width of the second Gaussian function, σ_{x_2} , should be 0.5 instead of 5.0. A corrected Table ?? is given.

Table 1: Parameters for the Gaussian functions added to the two-dimensional test potential.

i	1	2
A_i	1.5	6.0
x_{0_i}	2.02083	0.8
y_{0_i}	-0.172881	2.0
σ_{x_i}	0.1	0.5
σ_{y_i}	0.35	0.7

The Gaussian widths should also be squared in the following Eq. 22, changing it from

$$G_i(x, y) = A_i e^{-(x-x_{0_i})^2/2\sigma_{x_i}} e^{-(y-y_{0_i})^2/2\sigma_{y_i}}$$

to

$$G_i(x, y) = A_i e^{-(x-x_{0_i})^2/2\sigma_{x_i}^2} e^{-(y-y_{0_i})^2/2\sigma_{y_i}^2}.$$

In Fig. 4, the force labelled as $\tilde{\mathbf{F}}^0$ should be $\tilde{\mathbf{F}}^\dagger$ to be consistent with the text.

Equations (15) and (17) should have $i - 1$ indices in the denominators,

$$\gamma_i = \frac{(\vec{F}_i - \vec{F}_{i-1}) \cdot \vec{F}_{i-1}}{\vec{F}_{i-1} \cdot \vec{F}_{i-1}}, \quad (15)$$

and

$$\gamma_i = \frac{(\vec{F}_i^\perp - \vec{F}_{i-1}^\perp) \cdot \vec{F}_i^\perp}{\vec{F}_{i-1}^\perp \cdot \vec{F}_{i-1}^\perp}. \quad (17)$$