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 1 is given.

Table 1: Parameters for the Gaussian functions added to the twodimensional 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,

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

and

$$\gamma_{i} = \frac{\left(\vec{F}_{i}^{\perp} - \vec{F}_{i-1}^{\perp}\right) \cdot \vec{F}_{i}^{\perp}}{\vec{F}_{i-1}^{\perp} \cdot \vec{F}_{i-1}^{\perp}}.$$
(17)