

Supplementary Information

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1 Derivation of the exact formula for $\alpha(\phi, \psi)$

The general formula for $\alpha(\phi, \psi)$ depends on four variables, namely $(\phi_i, \phi_{i+1}, \psi_i, \psi_{i+1})$. The expression for $\tan(\alpha)$ is a rational function of fourth order trigonometric polynomials in the mentioned variables. Each coefficient is, in turn, a polynomial in $\sin(\gamma_1)$, $\cos(\gamma_1)$, $\sin(\gamma_2)$, $\cos(\gamma_2)$, $\sin(\tau)$ and $\cos(\tau)$. The whole exact, symbolic, expression contains hundreds of terms, and is definitely not manageable. However, by substituting the numerical values of the parameters namely $\gamma_1 = 20.7$ deg, $\gamma_2 = 14.7$ deg and $\tau = 111$ deg, one can obtain a numerical expression (that we called “actual”) that is implementable in a computer code.

In the approximation $\phi_i = \phi_{i+1}$ and $\psi_i = \psi_{i+1}$ a manageable expression can be obtained at the second order in γ_1 , γ_2 and $\tau - \pi/2$:

$$\alpha = \phi + \psi + \pi + \gamma_1 \sin(\psi) + \gamma_2 \sin(\phi) + \frac{1}{4}\gamma_1^2 \sin(2\psi) + \frac{1}{4}\gamma_2^2 \sin(2\phi) + \gamma_1\gamma_2 \sin(\phi + \psi) - \gamma_1(\tau - \pi/2) \sin(\psi) - \gamma_2(\tau - \pi/2) \sin(\phi)$$

Careful attention needs to be paid to keep the value of alpha in the $[-\pi; \pi]$ interval. We observe that $\tau - \pi/2$ appears only in the second order mixed terms, coupled with γ_1 and γ_2 . In its linear approximation, this expression returns eqn. (2) (see main text), where the dependence on τ is absent.

In fig. 1, we compare the performance of the second order formula and the first order formula plotting the approximate values of α versus the “actual” ones. As can be seen from the graphs, the second order formula is an excellent approximation of the desired value for α , (relative error of $\sim 1.4\%$, on a suitably populated configurational ensemble). However, the first order formula can also be a good approximation, if the values of the parameters are “optimized” to reproduce the true values. Using the optimized values of the parameters, we obtain, on the same ensemble, a relative error of $\sim 3.7\%$.

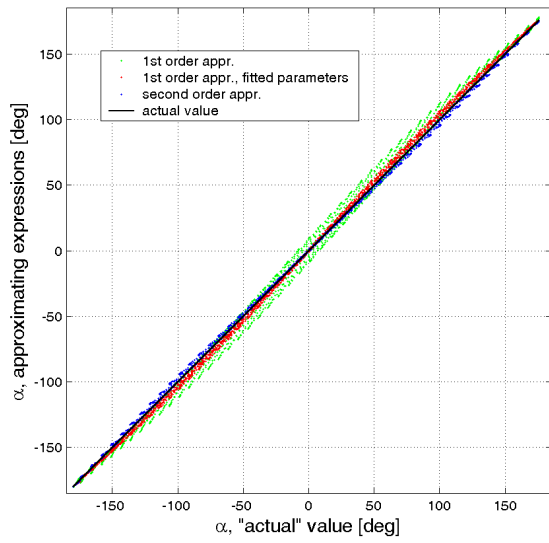


Figure 1: Approximate values of α versus the exact ones, evaluated on a set of ϕ, ψ pairs evenly spaced in the ϕ, ψ plane. Black line: explicit numeric formula, used as reference. Blue line: second order formula, using the actual values of the parameters: $\gamma_1 = 20.7$ deg, $\gamma_2 = 14.7$ deg, $\tau = 111$ deg. Green line: first order formula using the actual values of the parameters. Red line: first order formula, using optimized values of the parameters, $\gamma_1 = 15$ deg, $\gamma_2 = 20$ deg