Nonlinear Double Day, Sevilla, May 17-18, 2004

Energy funnelling and bubble generation in a bent and twisted DNA model

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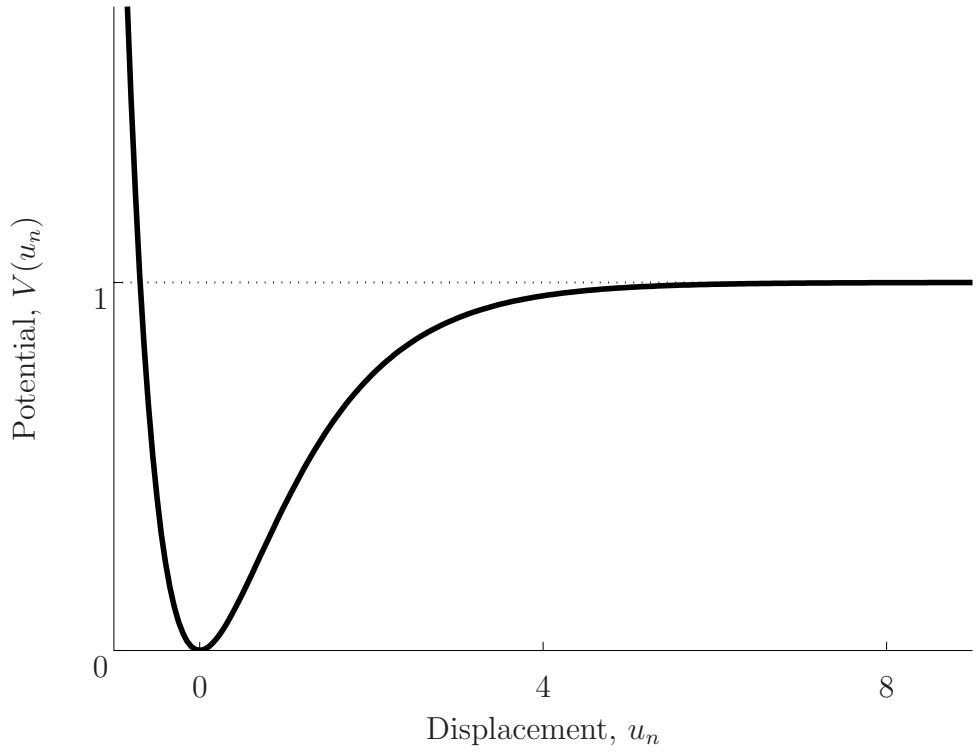
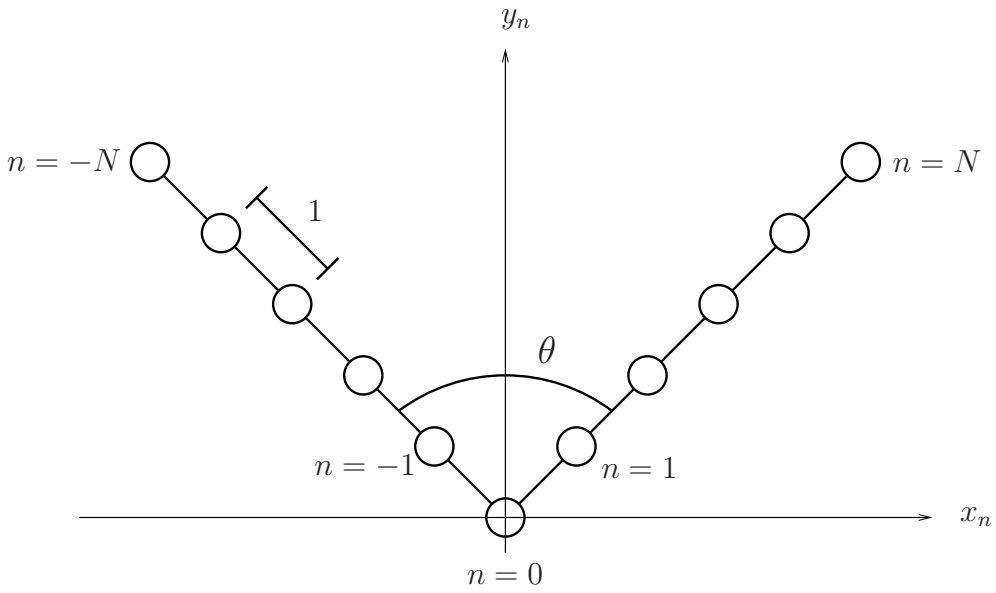
A plane bent chain of Morse oscillators with long-range dispersive interaction is first considered. Moving localized oscillations may be trapped in the bending region. Thus the chain geometry acts like an impurity. Energy funelling is observed in the case of random initial conditions modelling temperature.

Secondly, an augmented model of the DNA molecule including long-range interactions between twisted base pair dipoles is presented. A mechanism for bubble generation is found for sufficiently strong values of the dipole interaction coefficient. The relationship between bubble generation, curvature and twist is investigated. An analytical approach supports the numerical results.

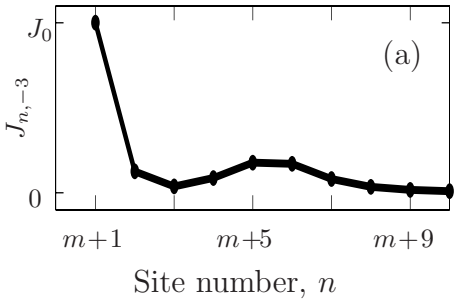
Morse potential

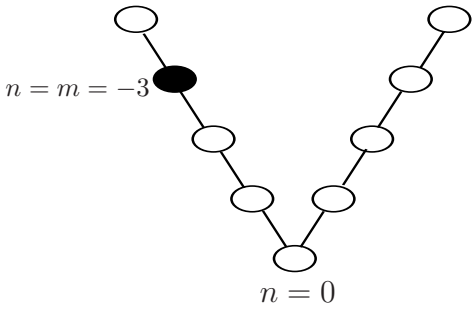


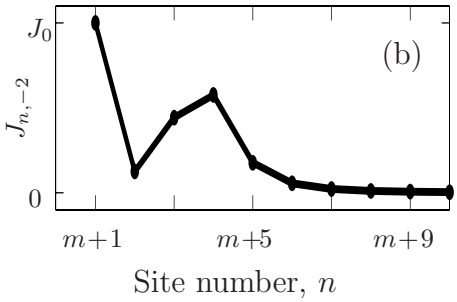
Chain geometry

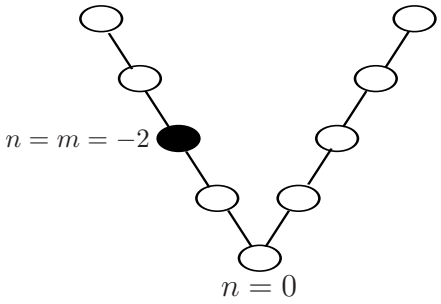


Dipole-dipole interaction

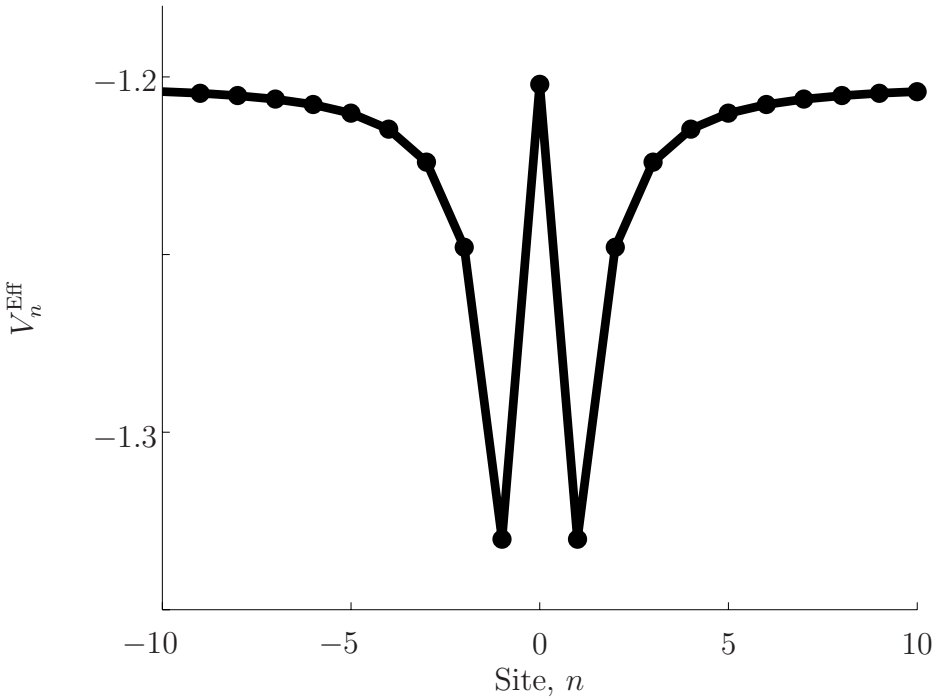




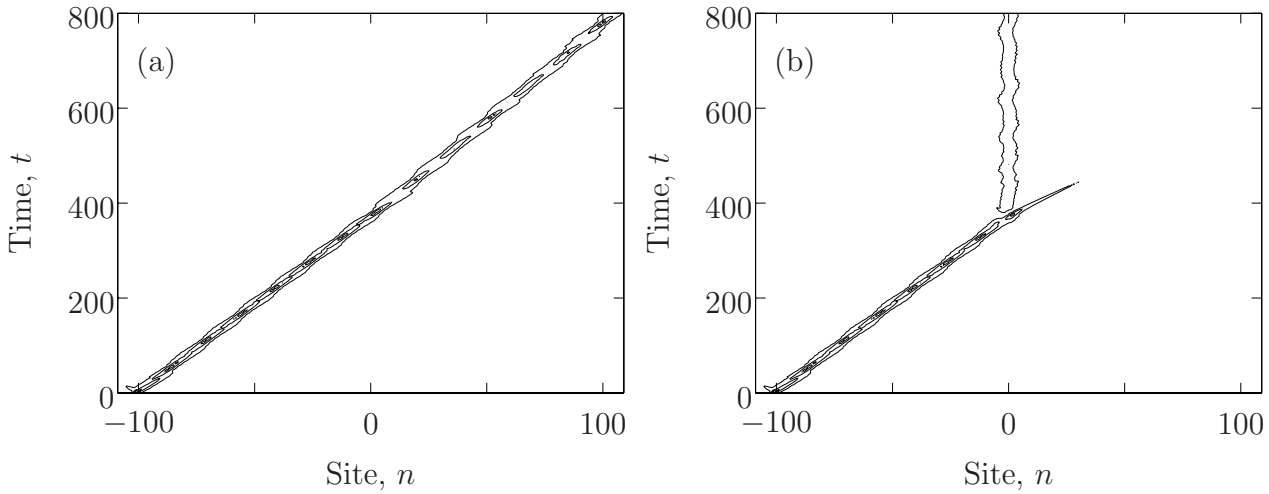




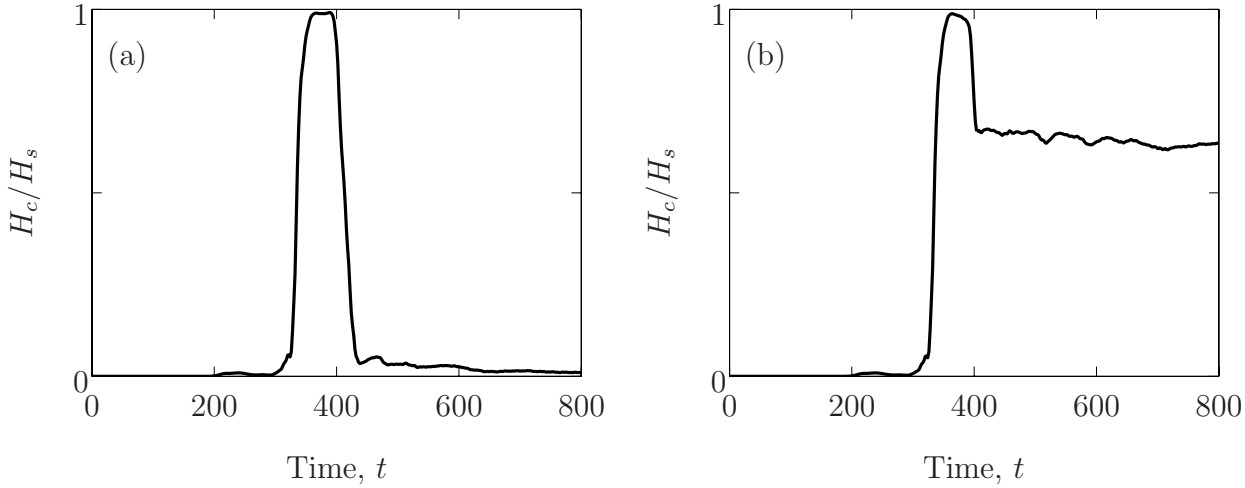
Effective potential



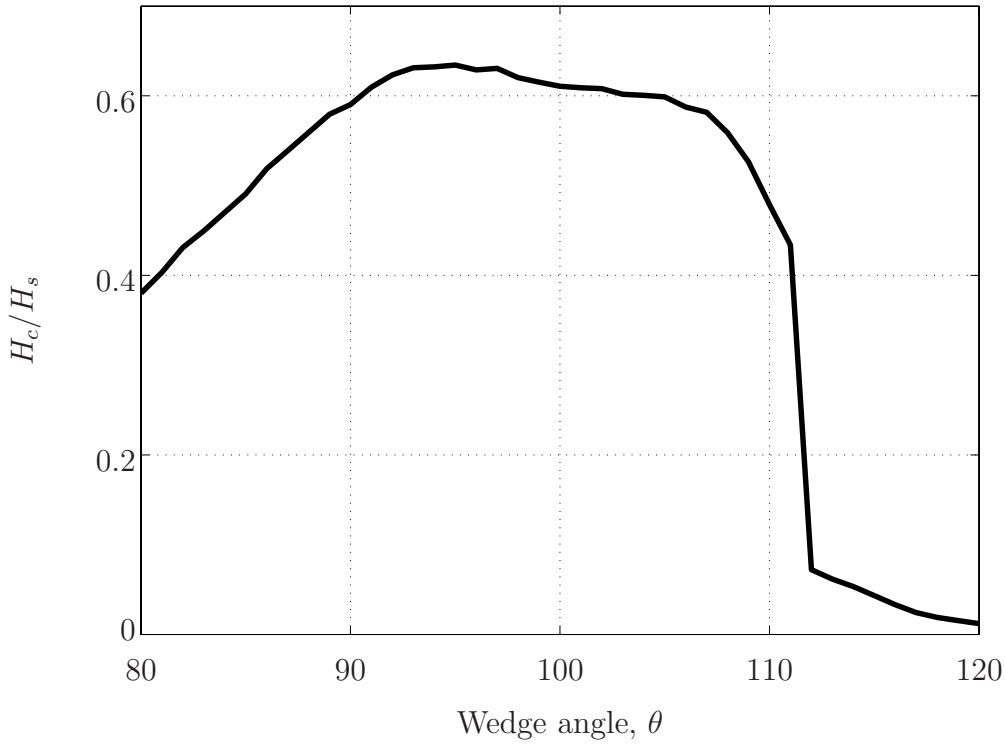
Hamiltonian density



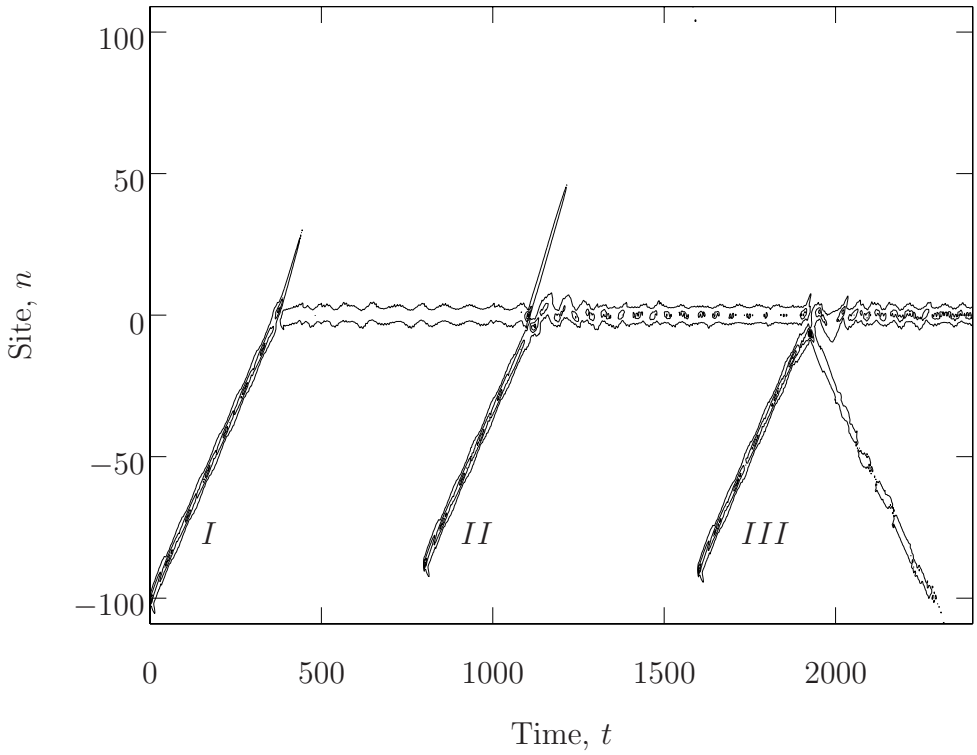
Central energy

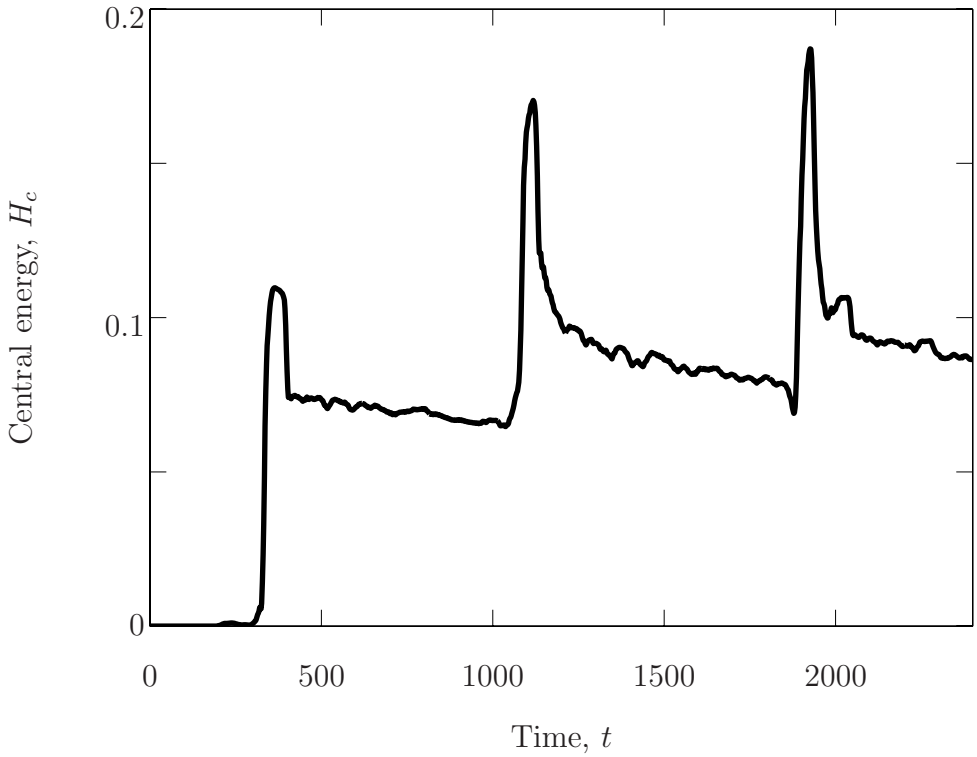


Central energy and wedge angle

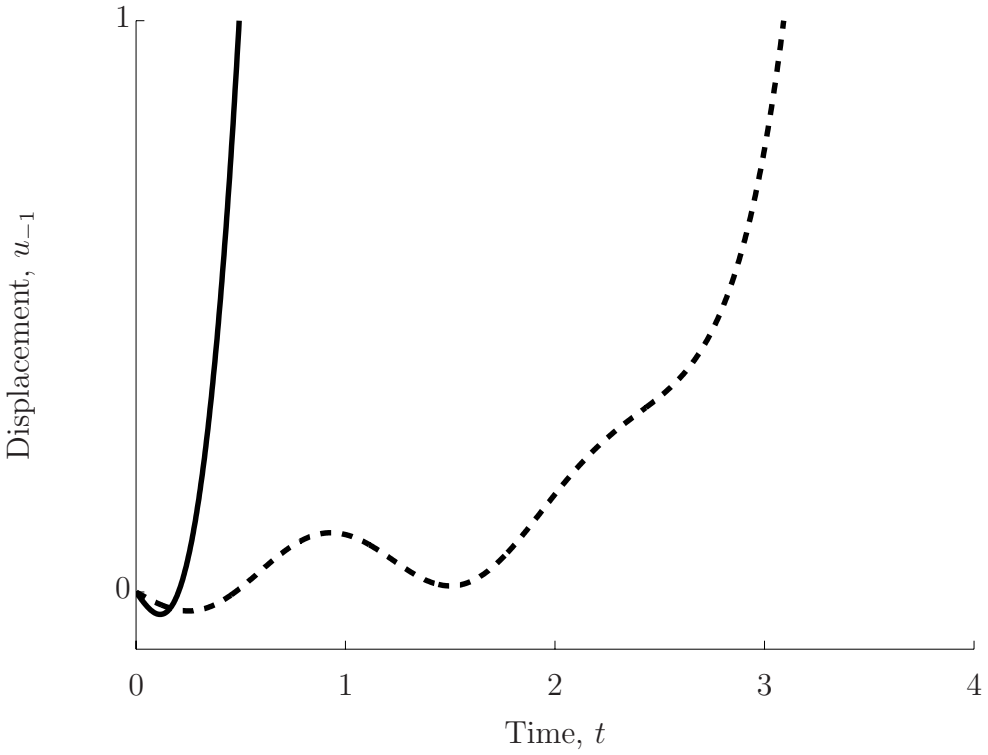


Multiple excitations



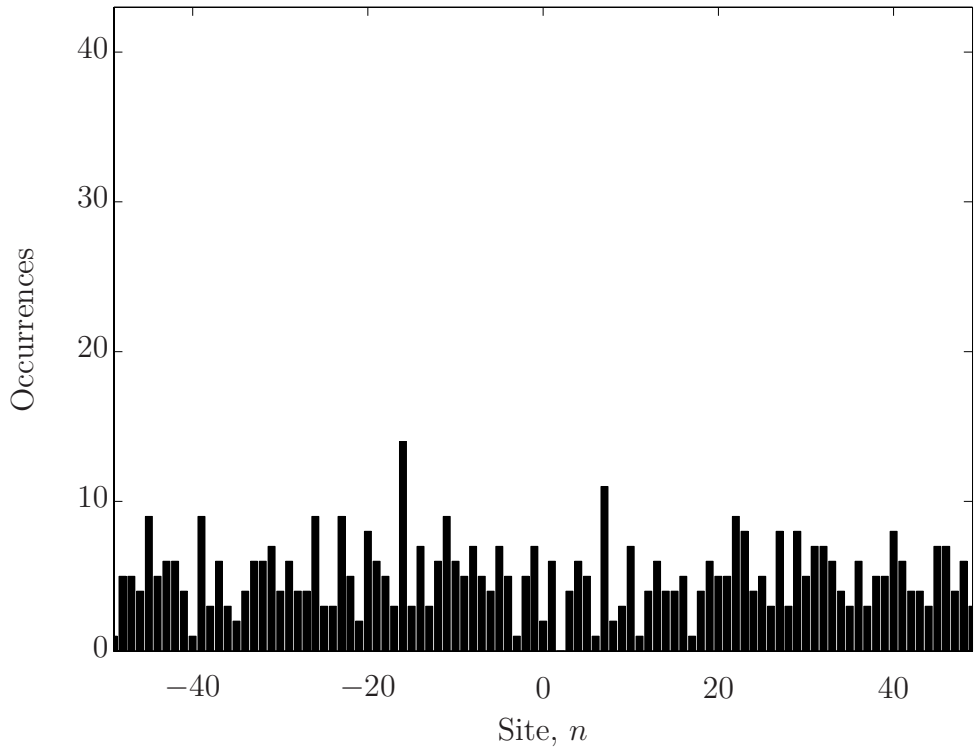


Amplitude increase

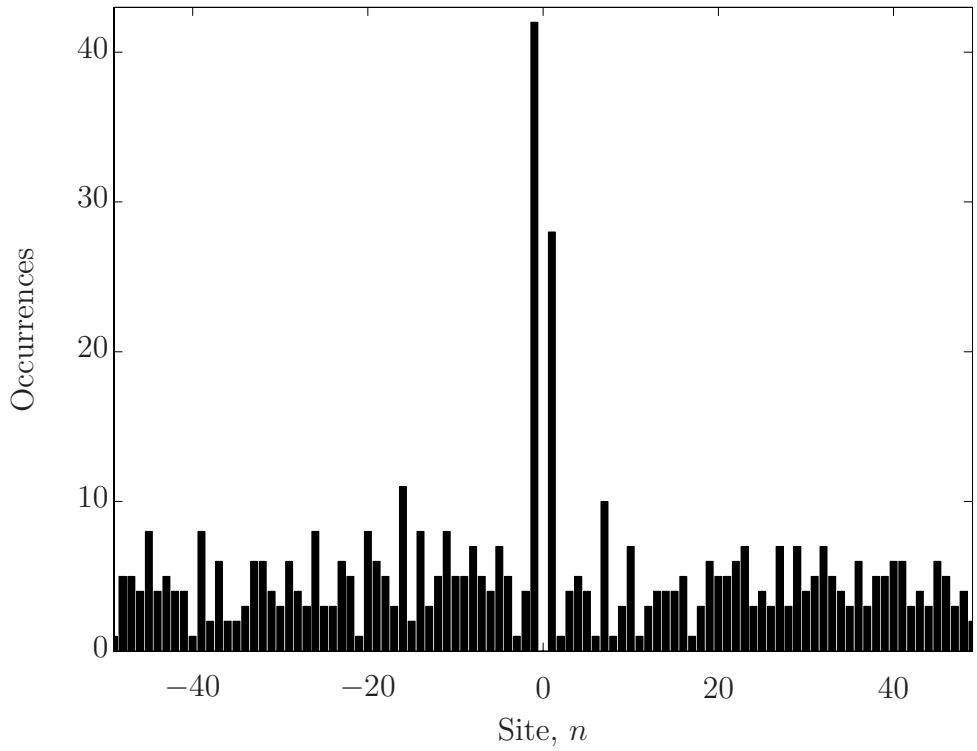


Occurrence sites

Straight chain, $\theta = 180°$.

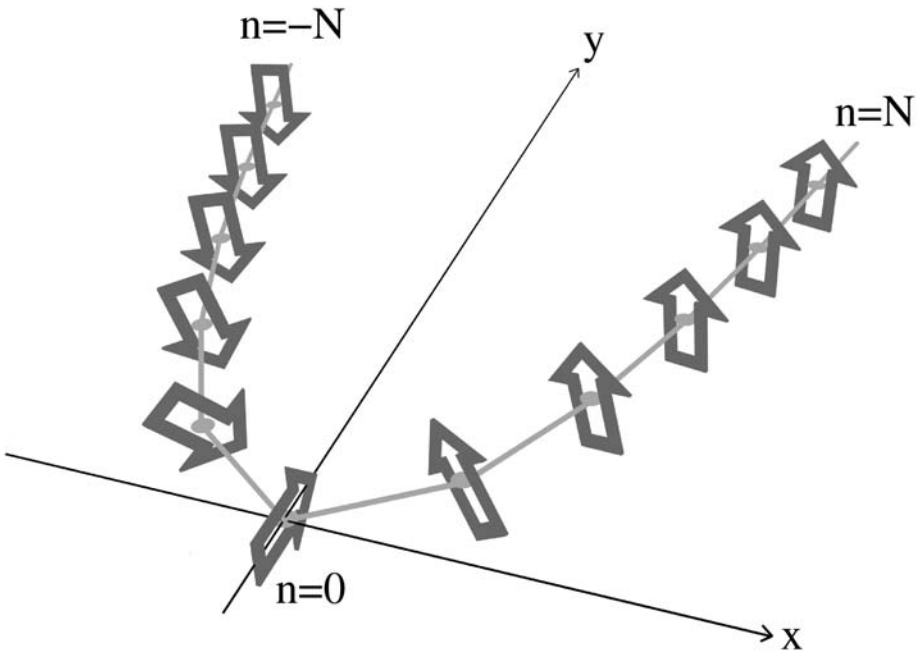


Bent chain, $\theta = 45°$.

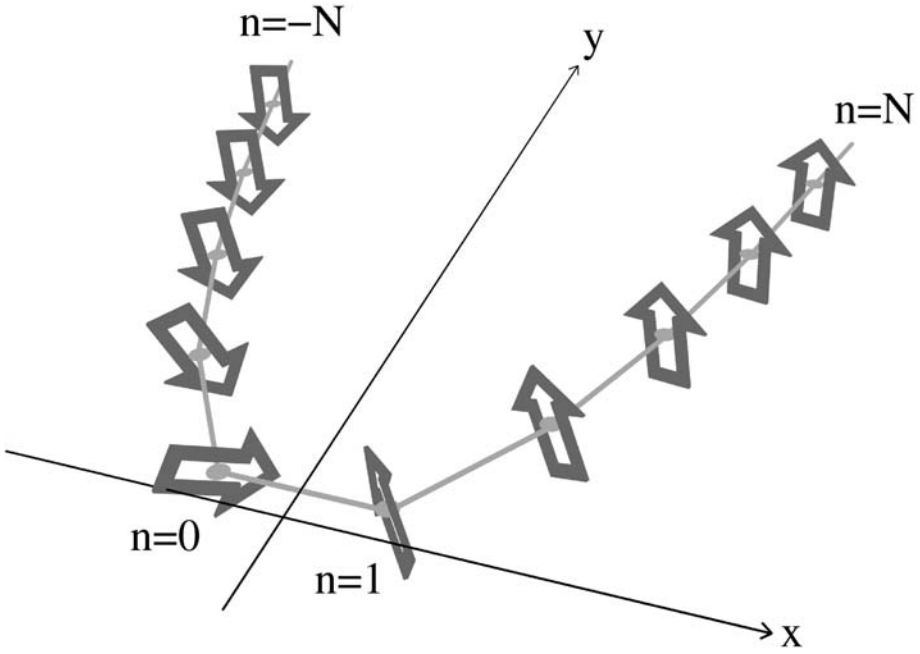


Chain geometry

On-site case, $\gamma = 0.\ \tau = 1.$

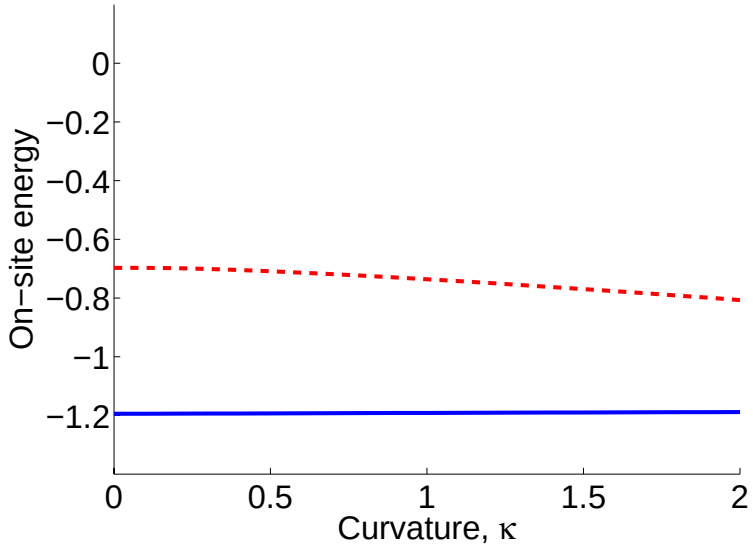


Inter-site case, $\gamma = \frac{1}{2}.\ \tau = 1.$



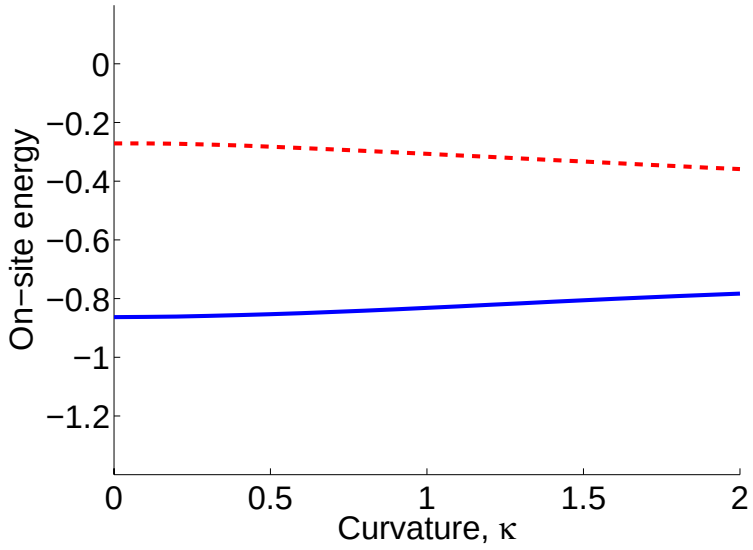
On-site energy for constant twist

On-site case. $\tau = 6$.



Sites $n = 0$ (solid) and $n = \{-1; 1\}$ (dashed)

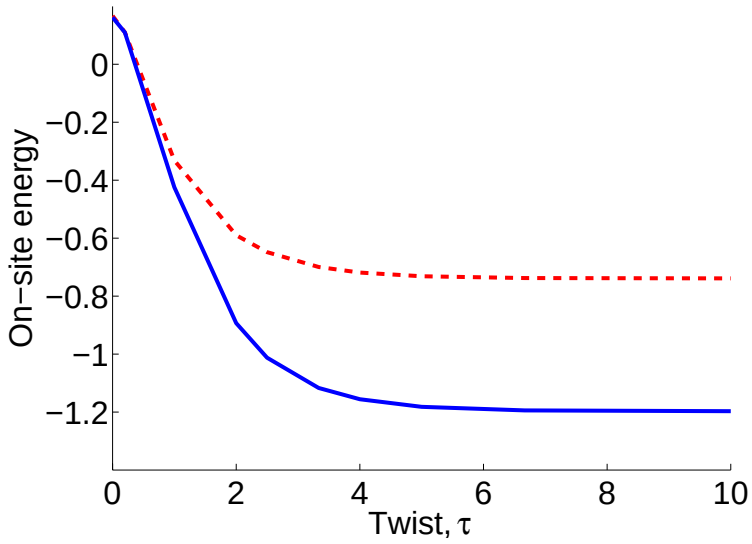
Inter-site case. $\tau = 2$.



Sites $n = \{0; 1\}$ (solid) and $n = \{-1; 2\}$ (dashed)

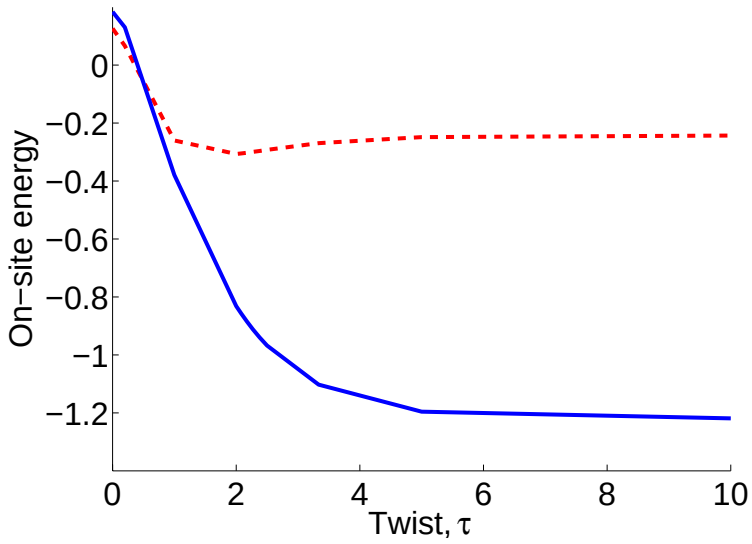
On-site energy for constant curvature, $\kappa = 1$

On-site case.



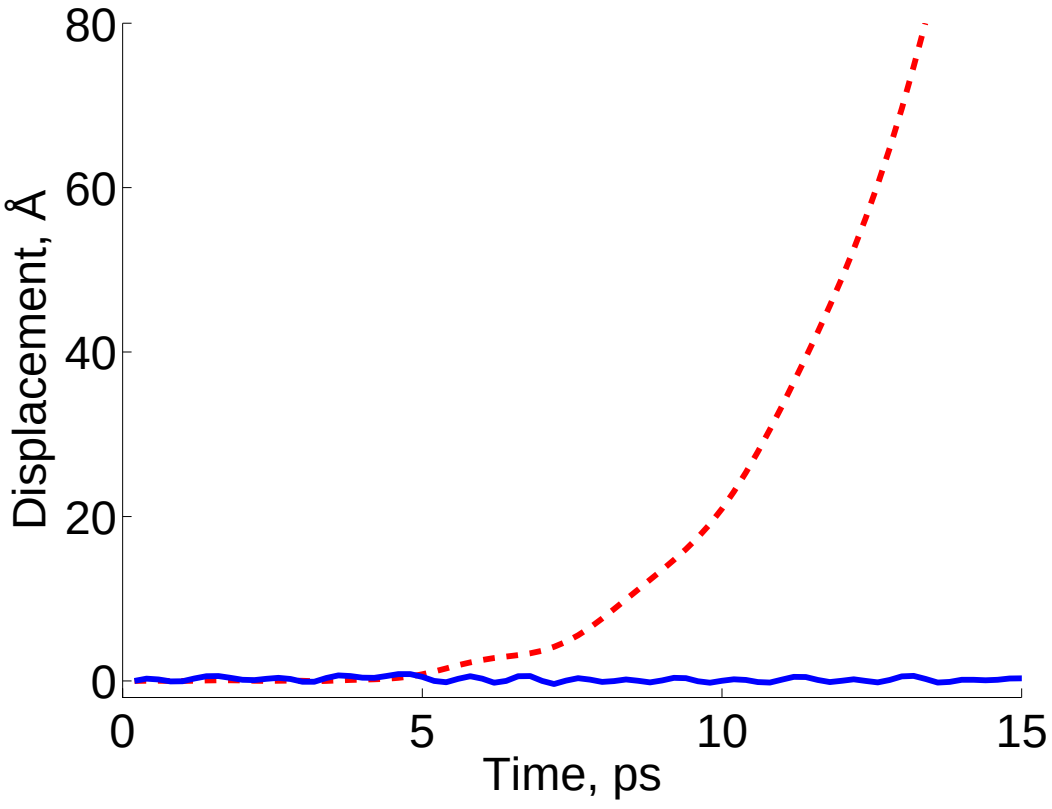
Sites $n = 0$ (solid) and $n = \{-1; 1\}$ (dashed)

Inter-site case.

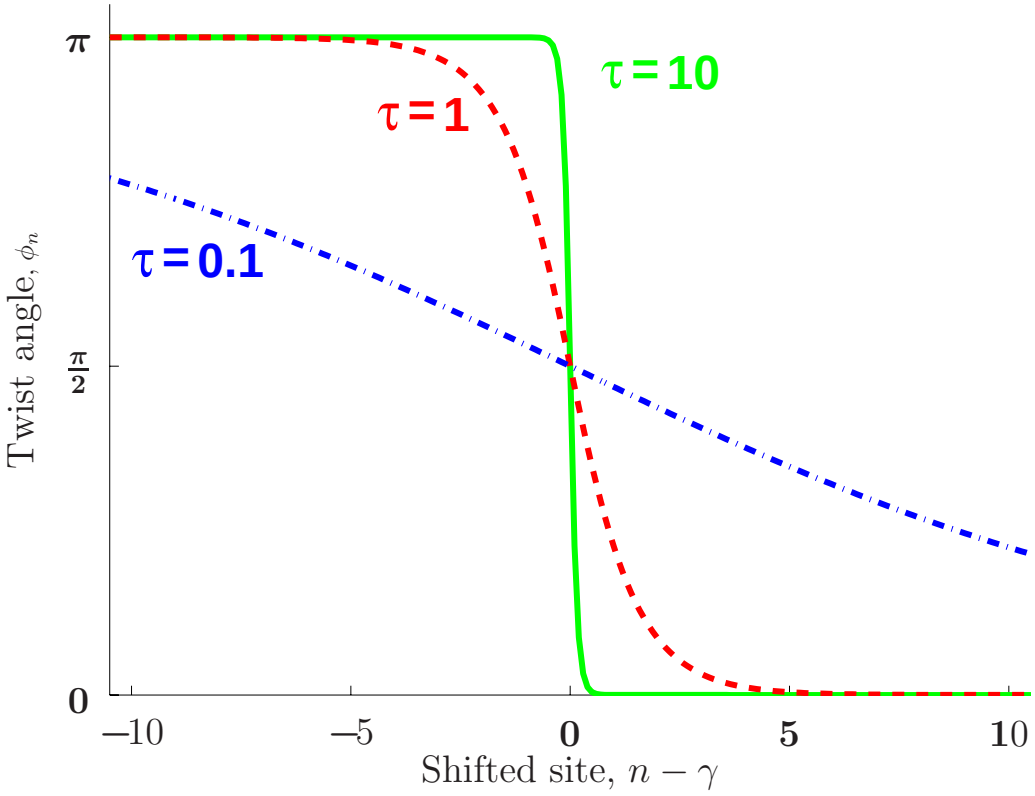


Sites $n = \{0; 1\}$ (solid) and $n = \{-1; 2\}$ (dashed)

Center site amplitudes, u_0, at $\kappa = 1.0$ for the on-site case.
$\tau = 2$ (solid) and $\tau = 6$ (dashed).

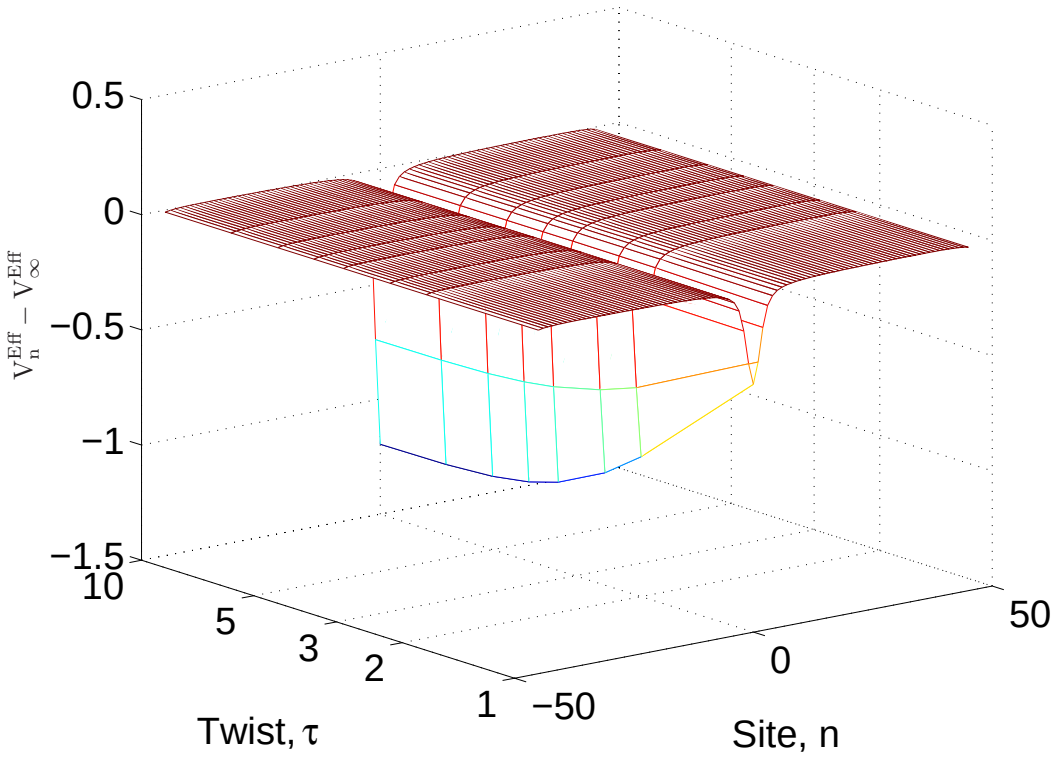


Twist angle, ϕ_n.

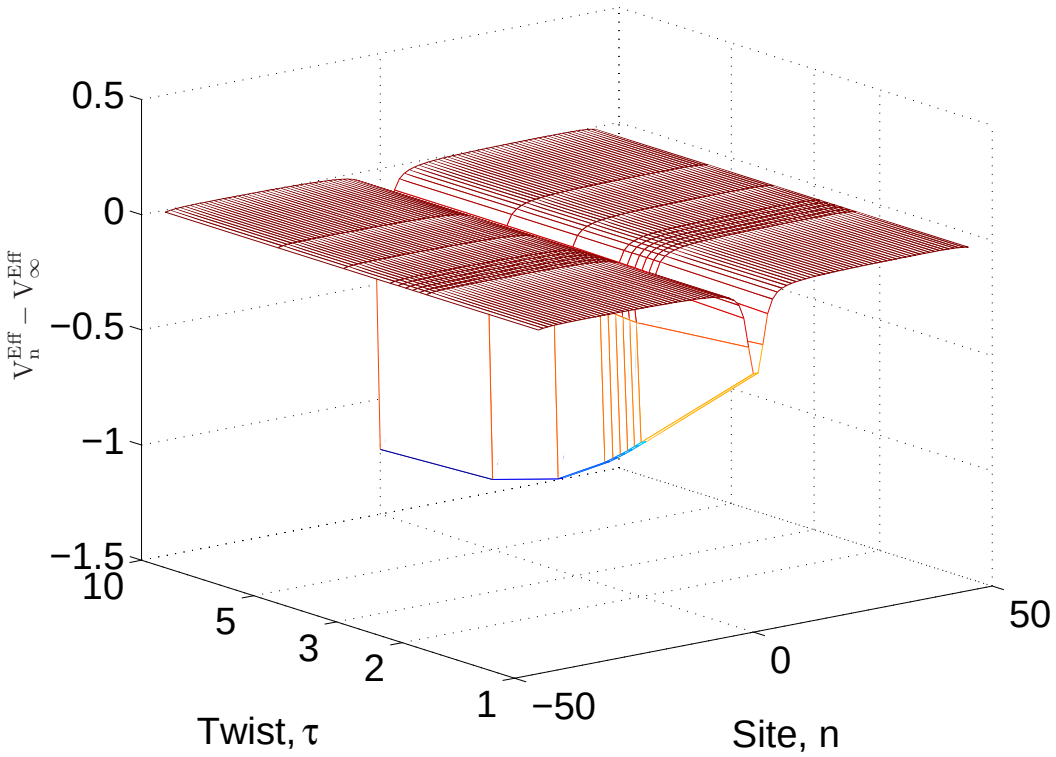


PL Christiansen et al, Nonlinear Double Day, Sevilla 2004

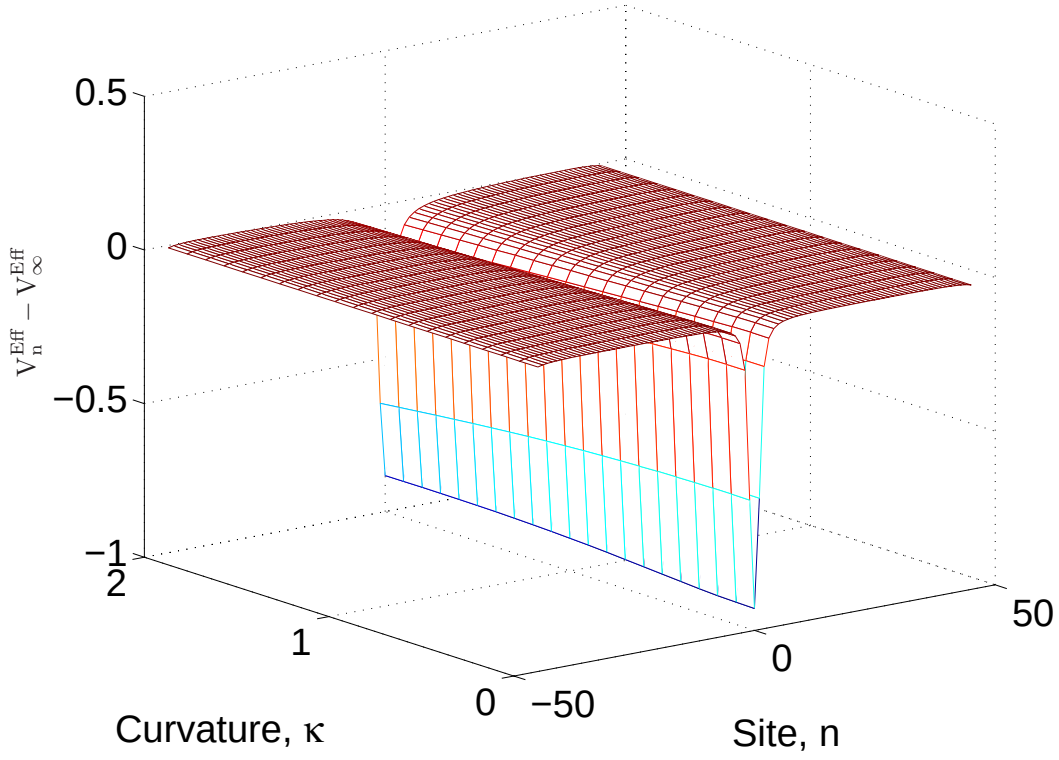
Effective potential for the on-site case at $\kappa = 1.0$.



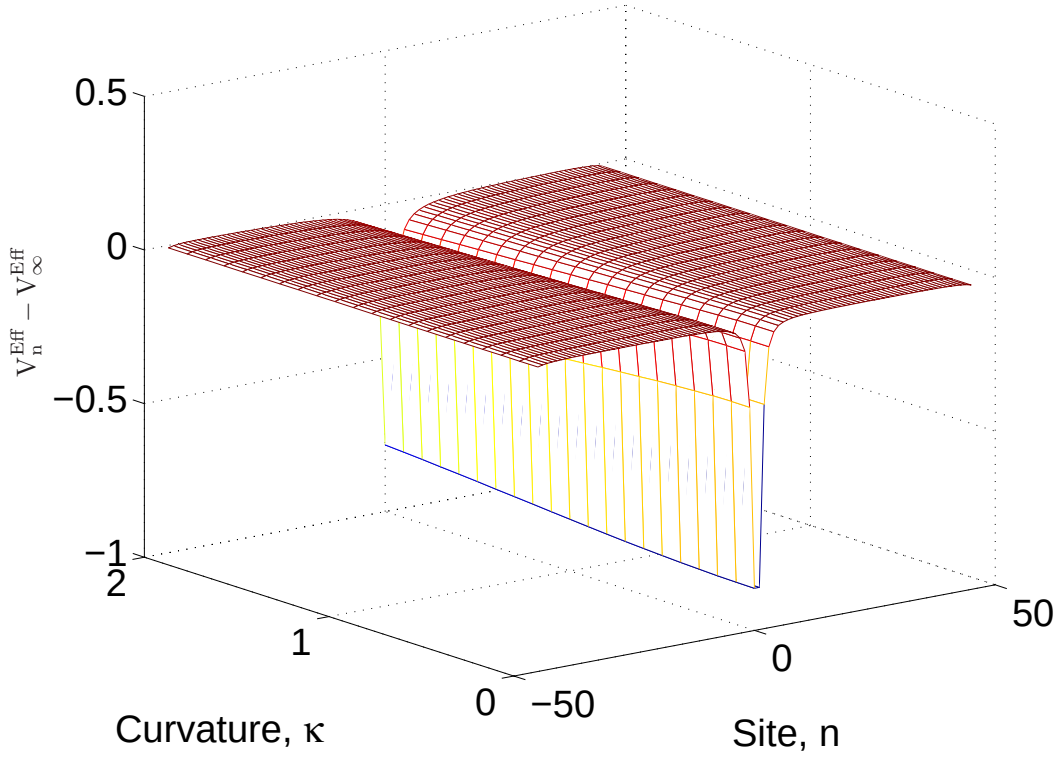
Effective potential for the inter-site case at $\kappa = 1.0$.



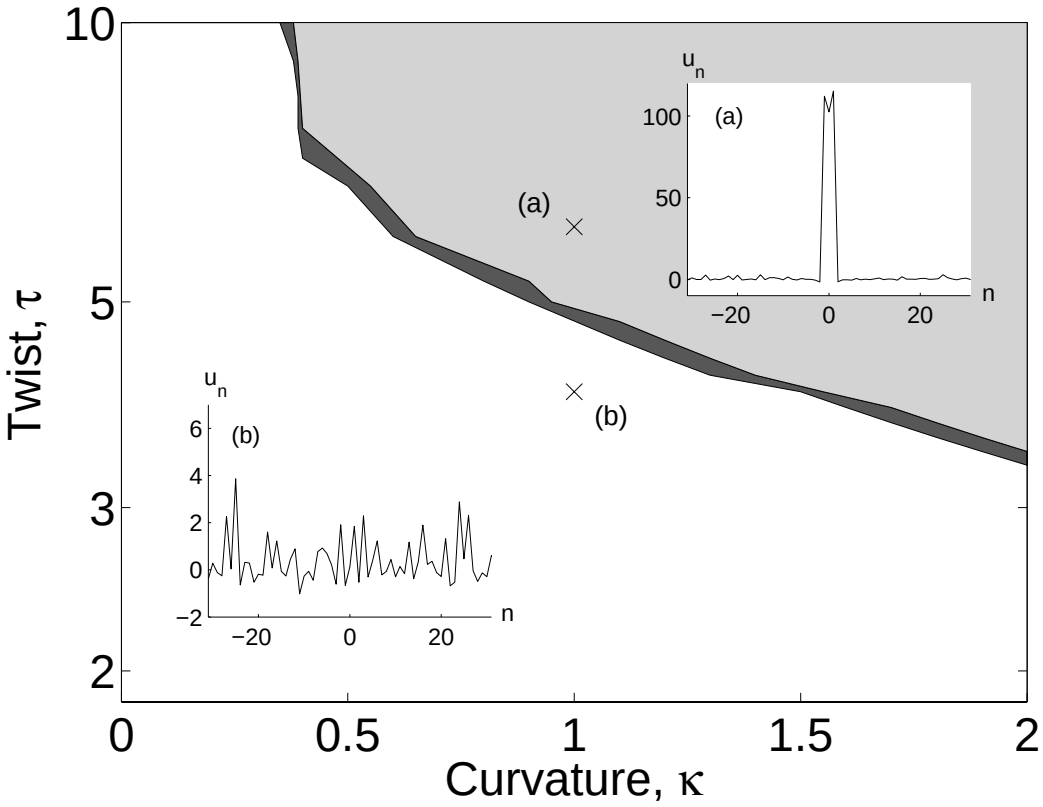
Effective potential for the on-site case at $\tau = 2.0$.



Effective potential for the inter-site case at $\tau = 2.0$.



Bubble generation in the on-site case.



Bubble generation in the inter-site case.