# EXTENSION OF A MODEL OF PROTEIN FOLDING TO THE MODELING OF NANOWIRES

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## Introduction

One-dimensional (1D) atomic-scale surface nanostructures are being extensively investigated as prospective building blocks (e. g., nanowires or nanomagnets) of future nanodevices [1,2]. Because at the atomic scale the conventional macroscopic fabrication techniques are inefficient, considerable attention attracted the phenomena of self-assembly and self-organization during coherent strained heteroepitaxial growth [1]. A major role in such a growth play the long range elastic forces caused by the lattice size misfit between the substrate and the growing overlayer. The positive misfit, in particular, causes the atoms sitting at nearby sites "push" each other in such a way that the addition of an atom to a contiguous chain is felt along the whole chain. Thus, the interactions in a 1D system with the misfit can be written in the following general form

$$H_{WSME} = \sum_{i=1}^{N} \sum_{l=1}^{i} V_i^{(l)} \prod_{k=i-l+1}^{i} n_k, \qquad (1)$$

where $n_k = 0, 1$ is the atomic occupation number of site $k$, the first sum goes over $N$ sites of a 1D system and $V_i^{(l)}$ is the interaction associated with a chain of length $l$ with its end being at site $i$. (To simplify notation, here and below we consider all parameters normally having the dimension of energy to be divided by $k_BT$.) Thus, in Eq. (1) the chain interactions are not homogeneous because they depend on the position of the chain in the system.

A model of type (1) with *homogeneous* interactions was derived and exactly solved by us in Refs. [3,4]. It turned out, however, that the general inhomogeneous model of this type was earlier proposed in connection with the problem of the protein folding by Wako, Saitô, Muñoz, and Eaton (WSME) and was solved exactly in Ref. [5] by a different method. This more general solution may be quite useful in technological simulations because in real devices the wires will not always traverse only homogeneous parts of the system but usually will experience the change of substrate or its doping, cross the steps, make turns, etc. To be fully realistic, however, Hamiltonian (1) should include other interactions, the most important being further neighbor pair interactions, such as the dipole elastic forces propagated by the substrate or the Coulomb interaction due to the charge transfer between the deposit and the substrate.

Below we generalize the iterative scheme of Ref. [5] to exactly solve the WSME (1) with a finite-range pair interactions.

## Generalized WSME model

*The model*

The extended WSME model we are going to solve has the Hamiltonian

$$H = H_{WSME} + \sum_{m=2}^{R} \sum_{i=m+1}^{N} w_i^{(m)} n_{i-m} n_i, \qquad (2)$$

where $w_i^{(m)}$ is the (inhomogeneous) pair interaction between two atoms separated by $m$ sites, $R$ the radius of the pair interactions. It has to be noted that while in 2D case the dipole forces are long range, in 1D case this is not so. Also the Coulomb interaction due to the charge transfer will be screened at large distances. So both interactions can be approximated to a desired accuracy by $R$ most important terms.

*Iterative solution*

The idea of the solution consists in representing the total partition function (PF) $Z^{(N)}$ of the system of size $N$ as the sum of $2^R$ partial PFs $Z_j^{(N)}$ corresponding to each of the $2^R$ configurations of the last $R$ sites. (It is convenient to chose $j = 0, \ldots, 2^R - 1$ so that its binary representation described the atomic occupation numbers.) This allows to establish an iterative scheme which would express the partial PFs for $N$-site system via the PFs of the $N-1$-site system. For simplicity we will illustrate the technique using the case $R = 2$ as an example. In the symbolic equation

$$\vec{Z}^{(N)} \equiv \begin{pmatrix} \circ\,\circ \\ \circ\,\bullet \\ \bullet\,\circ \\ \bullet\,\bullet \end{pmatrix}^{(N)} = \begin{pmatrix} \circ \\ \bullet \end{pmatrix} \times \begin{pmatrix} \circ\,\circ \\ \circ\,\bullet \\ \bullet\,\circ \\ \hline \bullet\,\bullet \end{pmatrix}^{(N-1)} \qquad (3)$$

the empty circles correspond to empty sites and the filled circles to the occupied ones. The multiplication sign on the right hand side symbolizes the process of adding an empty site and then an occupied one to the system consisting of $N-1$ sites. The empty site does not interact with anything so the statistical factor corresponding to it is unity and the contributions of the terms with the empty end site into $\vec{Z}^{(N)}$ are trivially found, as can be seen from the first two of the following set of equations:

$$Z_0^{(N)} = Z_0^{(N-1)} + Z_1^{(N-1)} \quad (4)$$

$$Z_1^{(N)} = Z_2^{(N-1)} + Z_3^{(N-1)} \quad (5)$$

$$Z_2^{(N)} = e^{-V_N^{(1)}} \left[ Z_0^{(N-1)} + e^{-w_N^{(2)}} Z_1^{(N-1)} \right] \quad (6)$$

$$Z_3^{(N)} = \sum_{l=2}^{N} e^{-E_N^{(l)}} Z_2^{(N-l+1)} / e^{-V_{N-l+1}^{(1)}}. \quad (7)$$

The addition of an occupied site is less trivial. While Eq. (6) causes no problems, in the last line in Eq. (3) one does not know what length has the chain to which the new atom is being added. Therefore, in (7) the chains of all allowed lengths (from $l = 2$ to $N$) has been accounted for ($E_N^{(l)}$ is the total energy of the chain of length $l$). Initialized by a system consisting of only one site, the above iterative scheme allows to compute the PFs for systems of any size.

*Quasi-1D systems*

A very important property of the extended WSME model consists in its ability to describe quasi-1D systems, i. e., the systems which have finite extent in the transverse direction, as shown in Fig. 1. As can be seen, the nearest neighbor sites on the 2D substrate became the second neighbor along the coordination line. In the extended model we can easily describe this situation by setting $V^{(2)} = w^{(2)}$ in Eq. (2). Now the chain interaction with $l = 3$ have the meaning of the cluster interactions within the trios of atoms on the equilateral triangle usually found in *ab initio* calculations. Furthermore, very large negative auxiliary trio interactions of this type can be added which would be exactly compensated by equally large but opposite in sign one atom interactions $V_{2i}^{(1)}$ *in the upper row* in Fig. 1. In this way only configurations satisfying the solid-on-solid restriction conventionally imposed on the surface structures will be allowed.

## Conclusion

We developed an iterative technique which provides the exact solution of the WSME model extended to account for finite range pair interactions. This extension allows for the treatment of elastic dipole forces and Coulomb interatomic interaction in (quasi)1D systems. Besides, this solution this opens a way for exact modeling of quasi-1D systems. To be of value, the radius of the farther neighbor interactions in the model $R$ should be sufficiently large. This should not pose significant problems for moderate values of $R$ because Eqs. (4)–(7) have simple structure so their derivation can be automated in case of $2^R$ reaching significant values.

From computational point of view our approach is rather economical. Because of the Eq. (7) its complexity is $O(N^2)$. This should be contrasted with the rejectionless Monte Carlo algorithm which in the presence of the long-range cluster interactions would require the calculations of complexity $O(N^2)$ *at every MC step*. And the results obtained will be only approximate.

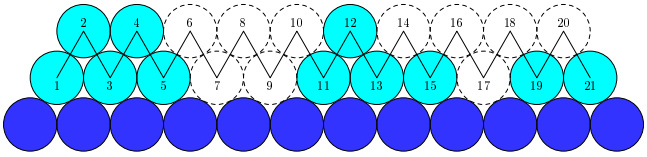


Fig. 1: Mapping of a quasi-1D atomic configuration on the 1D lattice gas model. The dashed circles correspond to empty cites. The circles in the bottom row correspond to substrate atoms. The configuration satisfies the solid-on-solid restriction and thus may model either the vertical growth in 1+1D or the growth on the steps of a vicinal surface.

## References


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