

Ground states of a one-dimensional lattice gas model with an infinite range nonconvex interaction. A numerical study

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Abstract

We consider a lattice gas model with an infinite pairwise nonconvex total interaction of the form

$$V(r) = \frac{J}{r^2} + A \frac{\cos(2k_F ar + \phi)}{r} .$$

This one-dimensional interaction might account, for example, for adsorption of alkaline elements on W(112) and Mo(112). The first term describes the effective dipole-dipole interaction while the other one the indirect (oscillatory) interaction; J , A , and ϕ are the model parameters, whereas k_F stands for the wavevector of electrons at the Fermi surface and a is a lattice constant. We search for the (periodic) ground states. To solve this difficult problem we have applied a novel numerical method to accelerate the convergence of Fourier series. A competition between the dipole-dipole and indirect interactions turns out to be very important. We have found that the reduced chemical potential μ/J versus A/J phase diagrams contain a region $0.1 \leq A/J \leq 1.5$ dominated by several phases only with periods up to nine lattice constants. Of course, the resulting sequence of phases (for fixed A/J) depends on the wavevector k_F and the phase shift ϕ . The remaining phase diagram reveals a complex structure of usually long periodic phases. We conjecture, based on the above

results, that quasi-one-dimensional surface states might be responsible for experimentally observed ordered phases at the (112) surface of tungsten and molybdenum.

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I. INTRODUCTION

There has been a widespread interest in structures and phase transitions in metal submonolayers chemisorbed on metal surfaces (e.g., for a review see Refs. 1,2). In particular, many alkaline, alkaline-earth, and rare-earth elements adsorbed on (112) faces of tungsten and molybdenum form, for low coverages, ordered structures consisting of linear chains of adatoms. Recently, a lattice gas model has been proposed to account for these structures.³ The results indicate that a formation of the linear chain submonolayer structures might be due to the competing (repulsive) dipole-dipole interaction and the long-range (oscillatory) indirect interaction between adsorbates. The indirect interaction was assumed to be mediated by the quasi-one-dimensional valence electronic states of the underlying substrate and was closely related to the existence of nearly flattened segments of the Fermi surface of W or Mo.^{2,3} It has been demonstrated explicitly that the resulting structures are very sensitive to a competition between the dipole-dipole and indirect interactions.³

It is the intention of this paper to understand the role of the interactions in determining the ordered structures. Since the general problem turns out to be quite complex, it is useful to focus on a simple model which contains the essential ingredients. We have considered an effective one-dimensional lattice gas model with the competing infinite range (convex) dipole-dipole and (nonconvex) indirect interactions and we study its ground-state phase diagrams. Our analysis is based on a novel numerical method to accelerate the convergence of Fourier series⁴ in order to take into account the interactions of the infinite range. In Sec. II we introduce a lattice gas model. The periodic ground states have been calculated numerically and the resulting phase diagrams are discussed in Sec. III. A possible role of surface states is considered in Sec. IV. The obtained results are summarized together with the concluding remarks in Sec. V.

II. THE MODEL

It is well known that the lattice gas models are quite useful in studying overlayer structures and their properties (e.g., Refs. 5,6). Here, we consider an effective one-dimensional lattice gas model with the following grand canonical ensemble Hamiltonian

$$H = \sum_i \sum_{r=1}^{\infty} V(r) n_i n_{i+r} - \mu \sum_i n_i , \quad (1)$$

where $n_i = 1$ or 0 depending on whether the i th site of the one-dimensional lattice is occupied or not by an adatom; $V(r)$ is an interaction between a pair of adatoms separated by distance r and μ is the chemical potential which controls the coverage of adatoms. The distance r is measured in units of a lattice constant.

We assume the pairwise total interaction $V(r)$ in the form

$$V(r) = \frac{J}{r^2} + A \frac{\cos(2k_F a r + \phi)}{r} . \quad (2)$$

The first term in Eq. (2) describes the effective dipole-dipole interaction in one dimension relevant to linear chain structures while the other one represents the indirect (oscillatory) interaction (see also Refs. 2,3); J , A , and ϕ are the model parameters, whereas k_F stands for the wavevector of electrons at the Fermi surface and a is a lattice constant of the lattice gas model.

In the following, we restrict ourselves to periodic configurations of n 's, i.e., there is a period p (positive integer) such that $n_{j+p} = n_j$ for any integer j . These are called p -periodic configurations of n 's.

Now, the energy per site of a given p -periodic configuration n_1, \dots, n_p can be written in the form

$$E[n_1, \dots, n_p] = \sum_{r=1}^p E_p(r) \sum_{i=1}^p n_i n_{i+r} - \mu \theta , \quad (3)$$

where

$$E_p(r) = J D_p(r) + A C_p(r) , \quad (4)$$

$$D_p(r) = \frac{1}{p^3} \sum_{s=0}^{\infty} \frac{1}{(s + r/p)^2}, \quad (5)$$

$$C_p(r) = \frac{1}{p^2} \sum_{s=0}^{\infty} \frac{\cos[x_p(s + r/p) + \phi]}{s + r/p}, \quad (6)$$

$$x_p = 2k_F a p, \quad (7)$$

$$\theta = \frac{1}{p} \sum_{i=1}^p n_i. \quad (8)$$

Let us note that the infinite range of the total interaction $V(r)$ requires the exact summations in Eqs. (5) and (6). This numerical problem will be discussed in the next section.

III. THE GROUND STATES

It is difficult to determine the ground states of the model Hamiltonian H rigorously because the total interparticle interaction $V(r)$ is *nonconvex* and we assume it to have the infinite range. This assumption seems to be necessary for the indirect (oscillatory) interaction is truly long-ranged. For a class of infinite-range interactions which are convex, positive, etc., it has been possible to find, in a one-dimensional case, all the ground states for any rational $0 < q/p < 1$, where q and p are integers with no common multipliers.⁷⁻¹⁰ The effects of nonconvexity on the ground states might be discussed, in principle, within a new general method of Griffiths and Chou.^{11,12} The method makes it possible to find the ground state configuration and the energy of one-dimensional systems by studying the corresponding nonlinear equation whose solution is an effective potential. Unfortunately, the method of Griffiths and Chou does not seem to work in the present case because of the infinite range of the slowly decaying total interaction [$V(r) \sim r^{-1}$ for large r] which makes it practically impossible to solve the eigenvalue equation. Note, however, that the method works well for interactions decaying exponentially.¹³

A. A numerical search for the ground states

In order to find the ground states we consider, instead of all possible configurations, only p -periodic configurations with the energy per site given by Eq. (3). Recently, we have proposed a numerical procedure to find such ground states.³ It consists of generating numerically all p -periodic configurations of n 's with $p = 1, \dots, p_{max}$ by using the bit representation of integers from the interval $[2^{p-1}, 2^p]$. The number of configurations could then be reduced by making use of the particle-hole symmetry⁵ as well as the translational and/or inversion symmetries. In this way, for example, the total number of p -periodic configurations for $p_{max} = 23$, 2^{23} , has been reduced to 181884 distinct configurations, i.e., by a factor of 46. Next, we check explicitly which configurations of n 's afford the minimal value to the corresponding $E[n_1, \dots, n_p]$ ($p = 1, \dots, p_{max}$), Eq. (3). However, this requires calculations of $D_p(r)$ and $C_p(r)$, Eq. (5) and Eq. (6), for $r = 1, \dots, p$ and $p = 1, \dots, p_{max}$. Here, we note that the infinite series result from the infinite range of the interparticle total interaction $V(r)$. It is not possible, to our knowledge, to calculate most of the sums of the corresponding infinite series analytically. Even a numerical calculation presents a problem due to a quite slow convergence of the series.

We have calculated numerically $D_p(r)$, Eq. (5), by using an analytic method of the convergence acceleration of the series.¹⁴ It is interesting to observe that for the p -periodic configurations we obtain the same contribution to $E[n_1, \dots, n_p]$, Eq. (3), by replacing $D_p(r)$ via $[D_p(r) + D_p(p-r)]/2$ (see Ref. 15). The numerical calculations of $C_p(r)$, Eq. (6) and Eq. (7), are more difficult for one can check explicitly that the standard methods to accelerate the convergence of the series do not work¹⁶ (especially for $mod_{2\pi} x_p$ close to 0 or 2π). To overcome this problem we have applied a novel method⁴ which introduces the so-called initial transformation and is followed by the ϵ algorithm for the associated complex Fourier series. The results are numerically exact (in double precision).

B. The ground-state phase diagrams

The ground-state configuration and the corresponding energy per site depend on the chemical potential, μ , and the model parameters, such as, J , A , ϕ , k_F , a , and p_{max} . In principle, calculations should be performed for p_{max} going to infinity to allow for any periodic structure. In practice, we have carried out calculations for $p_{max} = 23$ as a compromise between the computing time and more refined results. Our numerical tests show that to understand the role of the nonconvex interparticle total interaction $V(r)$ in determining the ground states, no additional significant insight can be achieved by extending the numerical computations to higher values of p_{max} .

The best way to discuss a competition between the effective dipole-dipole and indirect interactions (or, equivalently, the role of nonconvexity) is to consider ground-state phase diagrams: the reduced chemical potential μ/J versus model parameters $A/J, \phi, k_F$. In the following calculations we shall assume $a = 3.16\sqrt{3}/2 \text{ \AA}$.

In constructing the phase diagrams we made use of the particle-hole symmetry, i.e., we present only the p -periodic ground states with $\theta \leq 1/2$ for $\mu < \mu_c = \sum_{r=1}^{\infty} V(r)$. Moreover, it is sufficient to consider only $k_F \in (0, \pi/a]$ because $E[n_1, \dots, n_p]$, Eq. (3), is periodic with respect to k_F (with a period of π/a) and it is invariant under the transformation: (k_F, ϕ) onto $(k'_F, \phi') = (\pi/a - k_F, -\phi)$. We also assume $\phi \in (-\pi, \pi]$.

Most of the μ versus x phase diagrams ($x = A/J, \phi, k_F$) turned out to have rather complex topology (up to 100 lines separating distinct phases). In order to determine precisely the regions of stability of phases we find sequences of the ground states at x and $x + \Delta x$, respectively. Usually, we assume Δx to be 1/50 of the whole range of x . Then, if the sequences are different, we make use of the bisection method, otherwise we continue our scan in x .

Now, we shall discuss the results with a special emphasis on the role the indirect (nonconvex) interaction plays in determining the ground states. As the reference results we consider the ground states for $A = 0$ which form, on the (θ, μ) phase diagram, the complete devil's

staircase with a rather involved fractal behavior.^{7–10}

We use standard notation for the ground state, i.e., q/p , which means q occupied sites in a unit cell of p sites. At the same time $\theta = q/p$ and, in the present study, we are not interested in what are the actual structures of the ground states. As we shall see, the calculated phase diagrams turned out to be quite complex. Therefore, in order to make them more clear we do not attach q/p labels to small regions of the phase diagrams usually corresponding to the ground states with larger periodicities.

1. Dependence on ϕ

We start with the nonconvex indirect interaction only ($J = 0$). A typical chemical potential μ versus phase ϕ/π ground-state phase diagram is shown in Fig. 1(a). The value $k_F = 0.82 \text{ \AA}^{-1}$ was chosen in view of the subsequent discussion. The broken line depicts the particle-hole symmetry line $\mu_c = \sum_{r=1}^{\infty} V(r)$. Here, 0/1 and 1/1 denote the low-density ($\theta = 0$) and high-density ($\theta = 1$) disordered ground-states, respectively.

Our results demonstrate clearly that the ground-state phase diagram is very sensitive to p_{max} for $0.5 < |\phi/\pi| < 1$. The part of the phase diagram is not “stable” against formation of the longer-periodic ground states for larger values of p_{max} . This particular behavior might be attributed to the fact that the function $C_p(r)$, Eq. (6) and Eq. (7), has the smaller value the closer $\text{mod}_{2\pi} x_p$ is to 0 or 2π . Thus, for a fixed p_{max} one can always find such $p > p_{max}$ for which the above condition is satisfied and this could be easily tested numerically. This is the reason for not discussing the part of phase diagrams.

The situation, however, is quite different for $|\phi/\pi| < 0.5$. Figure 1(a) shows that apart from the 1/2 and 1/3 ordered ground states there is a coexistence of the low-density ($\theta = 0$) and high-density ($\theta = 1$) disordered ground states. It is due to an effective attraction of the nonconvex indirect interaction. Inclusion of the repulsive convex dipole-dipole interaction changes this part of the phase diagram and some of the typical results are presented in Fig. 1(b). The dependence on ϕ is very important from a physical point of view because by

changing its value one can induce distinct sequences of the ground states. It is worth to notice that relatively large parts of the phase diagram, Fig. 1(b), are occupied by the ground states having low periodicities p , like 2, 3, 4, 5, or 6.

2. Dependence on A/J

The ground states depend on the strength of the nonconvex interaction A in a crucial way. This is demonstrated explicitly in Fig. 2(a) and Fig. 2(b). It is easy to see that the devil's sequence of the ground states ($A = 0$) is destroyed even for a small value of A/J , leaving only a number of lower periodic phases. More precisely, for $0.1 < A/J < 1.5$, the phase diagram is dominated by such phases. The numerical tests show that this topology is not affected by p_{max} . We believe that this is a “physical” region which might account for the ground-state structures and/or phase transitions in linear chain structures,¹⁻³ at least. Indeed, following our previous model of adsorption of lithium on W(112) and Mo(112) (see Ref. 3), we have estimated A/J for the two cases. We find $A/J \approx 0.3$ ($\phi \approx 0.3\pi$) for Li/W(112) with $k_F = 0.41 \text{ \AA}^{-1}$ and $A/J \approx 1.3$ ($\phi \approx -0.1\pi$) for Li/Mo(112) with $k_F = 0.47 \text{ \AA}^{-1}$. The corresponding sequences of the ground states have been denoted by the vertical dashed-dotted lines in Fig. 3(a) and Fig. 3(b), respectively. A very good agreement with previous results, Ref. 3, is in favour of the present one-dimensional model as far as the linear chain structures are concerned. Let us observe that for sufficiently large A/J the lower periodic phases are replaced by a number of the narrow ground states having large periodicities.

3. Dependence on k_F

This dependence is important because of the underlying physics leading to the indirect interaction (virtual bulk and/or surface electronic states).^{1,2} However, to get more insight into properties of the ground states one can consider k_F as a parameter and some of the results obtained for such a case are shown in Fig. 4 and Fig. 5.

Note that the upper scale, $\pi/a - k_F$, is related to the lower one, k_F , for $\phi = 0$. And, as before, the broken line denotes a particle-hole symmetry line. The ground-state phase diagram for the nonconvex indirect interaction only is shown in Fig. 4. Let us note that for $k_F \rightarrow 0$ one restores the devil's staircase because the interaction $V(r)$ becomes convex. Modifications to the phase diagram in Fig. 4 due to a competition between the interactions are presented in Fig. 5(a) and Fig. 5(b). Again, the presented phase diagrams show relatively large, stable regions of the ground states with lower periodicities. It can be seen that the role of the phase, ϕ , is to “shift” the corresponding phase diagram as shown in Fig. 5(a) and Fig. 5(b).

IV. A POSSIBLE ROLE OF SURFACE STATES

The obtained results suggest that a given sequence of the ground states could be described by different k_F wavevectors with appropriately chosen amplitudes A and phases ϕ . For example, one of the possibilities may be connected with the transformation $(k'_F, \phi') = (\pi/a - k_F, -\phi)$ for a fixed value of A (see also Sec. III). This observation leads us to a conjecture concerning a possible role of *surface states* in understanding a formation of the linear chain structures. Indeed, the indirect interaction between adatoms via virtual electrons from quasi-one-dimensional surface states has the same form, as we have already discussed (cf. Refs. 2,17–19). Now, the wavevector k_F is determined from the Fermi lines corresponding to partially filled surface-state band(s) and it can be different from the one relevant to the bulk electronic states.

To our best knowledge, there are neither experimental nor theoretical results concerning partially filled surface-state band(s) of the (112) surface of W and Mo. However, a recent suggestion by Tosatti²⁰ as well as interpretation of the LEED data obtained for adsorption of lithium on W(112), Mo(112), and Ta(112)²¹ lead to a conclusion that surface states or surface resonances could exist on W(112) and Mo(112). Of course, this conclusion has to be confirmed by the corresponding experiments and selfconsistent calculations following, for

example, Ref. 22.

In general, the adsorption can substantially influence surface states by changing their band(s) structure and/or the surface Brillouin zone. Consequently, the form of the indirect interaction mediated by surface states² could be changed. In our case, however, we study the model relevant to the low coverage linear chain structures and it is plausible, therefore, that the influence on surface states can be neglected.

Our results seem to be consistent with the conjecture concerning surface states. For example, in order to explain a Sr/Mo(112) adsorption system at low coverages, one has to consider $k_F \approx 0.82 \text{ \AA}^{-1}$ and not the wavevector $k_F = 0.47 \text{ \AA}^{-1}$ connected with the bulk electronic states. Also a Li/Mo(112) system could equally well be described by using $k_F \approx 0.82 \text{ \AA}^{-1}$ [see Fig. 2(a)].

V. DISCUSSION AND CONCLUSIONS

The paper analyses the ground states of a one-dimensional lattice gas model with the infinite range pairwise interaction being the result of a competition between the convex dipole-dipole and nonconvex indirect interactions. The ground-state phase diagrams depend on three model parameters: A/J , k_F , and ϕ . Their complicated, at first sight, structures have, however, quite simple explanation. Indeed,

1. By increasing A/J from 0.1 to 1.5 (approximately) one *reduces* sequences of the ground states to those which contain only several lower-periodic phases. These phases exist in relatively large, stable regions, whereas the longer periodic phases enter only in narrow ranges in between (Figs. 2 and 3).
2. The wavevector, k_F , changes sequences of the ground states.
3. The change in the phase, ϕ , results effectively in a “shift” of the corresponding phase diagram in k_F [Figs. 5(a) and 5(b)].

It seems that the present model can describe qualitatively linear chain phases adsorbed at low temperatures on the (112) face of W or Mo.³ The model parameters have a definite physical meaning and distinct sequences of phases (the ground states) are governed by different values of A/J and ϕ which, in turn, depend on a particular adsorbate-substrate system. Of course, the wavevector k_F is closely related to a mechanism of the indirect interaction (bulk or surface electronic states).

Different linear chain structures, observed experimentally at 77 K on the (112) surface,² might be described within our model by assuming one value of k_F with different values of ϕ . The remaining parameter, A/J , is to be taken from the range (0.1, 1.5). For Li/W(112) and Li/Mo(112) we can estimate A/J (note that ϕ and k_F are chosen as in Ref. 3) and the results are shown in Fig. 3(a) and Fig. 3(b), respectively. A qualitative agreement is in favour of the present simplified model. It is interesting to observe that for $k_F = 0.82 \text{ \AA}^{-1}$ (or $\pi/a - 0.82 \text{ \AA}^{-1}$), Fig. 5(a), we find the ground states with periods 2, 5, and 9 (in units of a lattice constant, a). The higher periodic ground states enter only in small intervals [see also Fig. 2(b)]. Our numerical study reveals that only small deviations of the model parameters, i.e., A/J , k_F , and ϕ , are possible in order to simulate the above sequence of the ground states. The case might be related to strontium submonolayer linear chain structures on Mo(112)² observed experimentally at $T = 77 \text{ K}$. Moreover, the physical mechanism behind the form of the indirect interaction does not seem to be connected with the virtual bulk electronic states^{23,24} because this would require $k_F = 0.47 \text{ \AA}^{-1}$. Instead, we conjecture that (one-dimensional) *surface* electronic states might be responsible for the ground states in the case of Sr/Mo(112). The wavevector $k_F = 0.82 \text{ \AA}^{-1}$ (or $\pi/a - 0.82 \text{ \AA}^{-1}$) would be determined by a band of surface states at the Fermi surface. (For details concerning the indirect interaction induced by surface states see, for example, Ref. 2). We would like to stress that the adsorption of lithium on W(112) could equally well be explained by the existence of surface states with the corresponding wavevector, k'_F and ϕ' related by the transformation $(k'_F, \phi') = (\pi/a - k_F, -\phi)$.

It would be interesting to verify the existence of partially filled surface state band(s) on W(112) and Mo(112). Moreover, a knowledge of the corresponding k_F could help to construct a more realistic two-dimensional model of phase transitions.

We believe that our results for the ground states can be treated as a starting point towards understanding experimental data at 77 K . A more advanced theory (Monte Carlo simulation, real-space or finite-size renormalization group, cf. Refs. 25,26) is needed to understand the (T, θ) phase diagram and to compare the underlying experimental data quantitatively. This, however, would also require extension of the present model to two dimensions to make it more realistic.

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FIGURES

FIG. 1. The ground-state phase diagrams. The broken line depicts the particle-hole symmetry line $\mu_c = \sum_{r=1}^{\infty} V(r)$. (a) μ vs ϕ/π for $J = 0$, $A = 1$, $k_F = 0.82 \text{ \AA}^{-1}$. (b) μ/J vs ϕ/π for $A/J = 0.5$, $k_F = 0.82 \text{ \AA}^{-1}$.

FIG. 2. The ground-state phase diagrams μ/J vs A/J for $k_F = 0.82 \text{ \AA}^{-1}$. (a) $\phi = -0.3\pi$. (b) $\phi = 0$.

FIG. 3. The ground-state phase diagrams μ/J vs A/J . (a) $\phi = 0.3\pi$, $k_F = 0.41 \text{ \AA}^{-1}$. The vertical dashed-dotted line at $A/J = 0.3$ corresponds to the case of Li/W(112). (b) $\phi = -0.1\pi$, $k_F = 0.47 \text{ \AA}^{-1}$. The vertical dashed-dotted line at $A/J = 1.3$ corresponds to the case of Li/Mo(112).

FIG. 4. The ground-state phase diagram μ vs k_F for $J = 0$, $A = 1$, and $\phi = 0$.

FIG. 5. The ground-state phase diagrams μ/J vs k_F for $A/J = 0.2$. (a) $\phi = 0$. (b) $\phi = -0.3\pi$.









