Fig. 1. \( ^{4}\text{He}^-/\text{U} \) rocking curve for the U surface peak near the (110) direction on the UC_{2}(111) surface. Experimental data are individual points with error bars. Solid curve (---) ideal bulk termination, no surface vibrational enhancement or correlation. Dashed curve (----) 0.19 Å outward relaxation of the U surface layer, surface vibrational enhancement of 1.2 and no correlation.

Summary Abstract: Relationship between many-parameter lattice gas systems and simpler models: Easy approximations for \( T_c \)

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While lateral interactions between chemisorbed atoms markedly affect many properties of the overlay, they resist quantitative measurement because of their small size relative to binding energies and diffusion barriers. A powerful way to probe the interactions is to measure the 2-d phase diagram of the overlay. The lateral interactions can then be treated as adjustable parameters in theoretical calculations (most often Monte Carlo) of the phase diagram.\(^{1-5}\) In this procedure it is typically necessary to limit the number of parameters (and values for each). Thus, it would be useful to have a method, given \( T_c \) for one (typically small) set of interactions, to estimate \( T_c \) for a system of the same symmetry for a different (typically larger) set. We have found such a scheme\(^{2-4}\) which is remarkably accurate for simple lattice gases for a wide choice of lateral interactions.

We describe the use of this method in terms of a \( c(2 \times 2) \) overlayer on a square lattice, as shown in Fig. 1. A \( c(2 \times 2) \) overlayer forms when there is a repulsive first neighbor interaction energy \( E_i \). If this is the only interaction, the problem translates directly into the zero field Ising model, for which \( E_i \approx 1.7 t_{T_c} \),\(^{6}\) shown as Onsager solution in Fig. 1. However, in real systems there are also longer range interactions, for instance, a second neighbor interaction \( E_{2n} \), as shown in Fig. 1. To determine the change in \( T_c \) caused by the addition of \( E_{2n} \), we consider the minimum energy required for an atom to move from an ordered site. As indicated by the \( \times \)'s in Fig. 1, the central atom can disorder most easily into a nearest neighbor site. If \( E_2 = 0 \), the energy cost for this move is \( 2E_{1n} \), since there is no repulsion from the newly formed vacancy at the "central" site. (In contrast, in mean field the-
Clearly, to use the excitation scheme the added interactions must not change the symmetry of the overlayers. In the range \(0.1 < E_2/E_1 < 1/2\) the impending symmetry change at \(E_2/E_1 = 1/2\) complicates the prediction of the minimum energy required to move an atom (i.e., multilayer moves evidently become important) causing the approximation to fail. The excitation scheme for \(E_2\) strongly attractive (\(E_2 > E_1\)) fails for a different reason. In this case the nearest neighbor repulsion becomes unimportant compared to the second neighbor attraction, and disordering into one of the sites marked by \(x\)'s is not favored over disordering into a random site. In short, the excitation scheme can be used only if the minimum-energy disordering move is significantly lower in energy than any other possible move.

The excitation scheme can be used for lattice gas systems with a variety of symmetries and hence with different sets of interactions than discussed here, for instance, the \((\sqrt{3} \times \sqrt{3}) R 30^\circ\) and \((2 \times 2)\) overlayers on a triangular lattice, the \((2 \times 2)\) on a honeycomb lattice, and the \((2 \times 1)\) on a bcc \((110)\) lattice. In addition, it can be used to estimate the effects of trio (non-pairwise) interactions\(^9\) on the phase diagram. A discussion of these applications, detailing their accuracy and their range of reliability, will be presented elsewhere.\(^9\)

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\(^9\)N. C. Bartelt, T. L. Einstein, and E. D. Williams (in preparation).