# Phase diagrams of surface structures from Bethe-ansatz solutions of the quantum sine-Gordon model

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Phase diagrams of uniaxial two-dimensional systems with commensurate, incommensurate, and liquid phases are derived by combining exact results for the quantum sine-Gordon model with the Kosterlitz-Thouless theory of melting. The phase diagram depends on the order of commensurability, $p$. In particular, for $p=3$ (the "chiral Potts" case), we conjecture that the phase diagram contains no Lifshitz point, in contrast to previous authors; for $p=1$, dislocations remove the original $CI$ transition completely.

It is well known that two-dimensional statistical mechanics can be formulated in terms of one-dimensional (1D) quantum field theory. Thus the phases of uniaxial surface structures can be analyzed from the ground-state properties of the one-dimensional sine-Gordon model.[1] The solitons of the sine-Gordon theory represent domain walls in the two-dimensional system driving the commensurate-incommensurate transition.[2] To obtain the full phase diagram, it has recently been emphasized[3-7] that it is necessary to include dislocations in the surface structure in order to assess the stability of the incommensurate phase against melting into a liquid phase.

We will here derive phase diagrams of systems which undergo transitions between commensurate ($C$), incommensurate ($I$), and liquid ($L$) phases. Our strategy is first to consider the $CI$ transition and the correlation functions in the $I$ phase in the absence of dislocations. To this end we use exact results for the sine-Gordon model with a finite density of quantum solitons which have recently been obtained by one of us[8] by means of the Bethe-ansatz solutions. The melting transition is then studied by adding the effects of dislocations through the theory of Kosterlitz and Thouless,[9] essentially "by hand." Though our results are only strictly valid in the limit of vanishing fugacity for dislocation pair creation (the "low vorticity" limit), we conjecture that the topology of the phase diagrams remains the same at finite vorticity. Our treatment is in the spirit of the treatment of the effects of in-plane anisotropy in the $XY$ magnet by José *et al.*[3]

The phase diagram depends strongly on the order of commensurability $p$ (the period of the surface structure measured in units of the substrate lattice constant). The theory gives a unified description for all values of $p$, and the results are summarized in Fig. 1. In certain limits, previous well-known results are reproduced. For $p>4$, a floating incommensurate phase always separates the $L$ phase and the $C$ phase, as found first by José *et al.*[3] For $p<\sqrt{8}$ (i.e., $p=1,2$) our findings agree with Villain and Bak[4] and Coppersmith *et al.*[5] who found that a liquid phase always separates the $C$ phase from the $I$ phase at finite tempera-

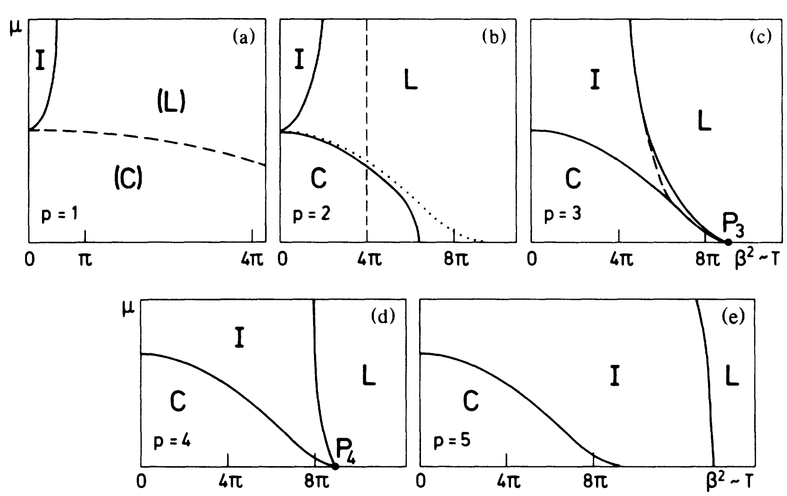


FIG. 1. (a)–(e) Phase diagrams derived by combining results from the quantum sine-Gordon model with the Kosterlitz-Thouless theory. The "pseudo"-$CL$ transition for $p=1$, and the alternative phase diagram (with Lifshitz point) of other authors for $p=3$, are indicated by broken lines. For $p=2$, the line corresponding to the exact solution of Ref. 6 is indicated by the broken line, and the dotted line is the $CI$ line in the absence of dislocations. The singular $p=3$ and $p=4$ (vector) Potts points $P_3$ and $P_4$ are also marked.

 

ture. For $p=3,4$, our results suggest that the $I$ phase everywhere separates the $C$ and $L$ phases except at an isolated $p=3$ or $p=4$ clock point. In particular, for $p=3$ (the "chiral" Potts model case) our phase diagram differs from the one suggested by Ostlund,[10] Selke and Yeomans,[11] Huse and Fisher,[12] and Howes, Kadanoff, and den Nijs,[13] who suggest a Lifshitz point where the $C$, $I$, and $L$ phases meet, as indicated by the broken line in Fig. 1. Though, as will be discussed, certain independent evidence is consistent with our $p=3$ result, modification by finite vorticity effects cannot be ruled out, and additional calculations (or experiments) should be performed.

For $p=1$, the dislocations have a second dramatic effect: The transition between the $C$ and $L$ phases is completely washed out at finite temperature, and only the transition line between the $I$ and $L$ phases remains.

In the absence of dislocations, the thermodynamic properties of a uniaxial system undergoing a $CI$ transition can be described by the ground state of the 1D quantum sine-Gordon Hamiltonian[1]

$$H=\int dx\,[\tfrac{1}{2}g\Pi^2+\tfrac{1}{2}g^{-1}(\vec{\nabla}\varphi-\mu)^2-\frac{\lambda}{T}\cos(p\varphi)]\ , \quad (1)$$

where $\mu$ is the natural misfit of the 2D system, $\lambda$ is the substrate potential, and $g$ is a measure of the temperature of the 2D system: $g=2\pi T$. $\varphi$ is a canonical field variable describing the position of the adsorbate relative to the substrate, and $\Pi$ is its conjugate momentum. The transition line separating the $C$ and $I$ phases has been calculated by Pokrovsky and Talapov[1]: For $\beta^2=p^2g\leq\beta_{\max}$ (i.e., $T\leq T_{\max}$), the model (1) has a commensurate phase at small $\mu$ which becomes incommensurate at $\mu=\pm\mu_C(\beta)$ (see Fig. 2). In terms of (1), the commensurate phase is a ground state with no solitons, and the incommensurate phase appears at $\mu=\mu_c$ where the excitation energy of the soliton vanishes. The limiting value $\beta_{\max}$ is found from the condition that the renormalized value of $\beta^2$ (renormalized by substrate potential effects) equals $8\pi$. Hence $\beta^2_{\max}=8\pi(1+\delta)$ and $T_{\max}=4(1+\delta)/p^2$, where $\delta$ is proportional to $\lambda$ at small $\lambda$.

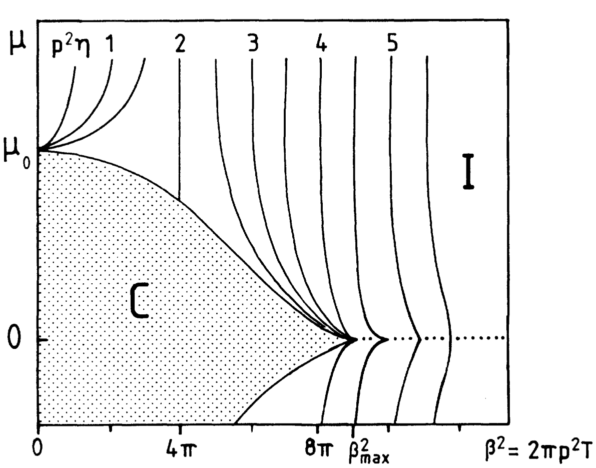


FIG. 2. Phase diagram derived from the quantum sine-Gordon model (1), as a function of misfit parameter $\mu$ and temperature. The commensurate ($C$) region and the lines of constant correlation exponent $\eta$ in the floating incommensurate ($I$) phase are shown. This represents a theory of the $CI$ transition that neglects the effects of dislocations on the $I$ phase; hence diagrams for different commensurability order $p$ may be scaled onto each other.

To determine the Kosterlitz-Thouless melting temperature for the $IL$ transition, we apply the results of Haldane[8] for the exponent $\eta$ which describes the decay of the density-density correlation function in the incommensurate phase. This is obtained from (1), without considering modifications due to finite vorticity effects.

Well inside the incommensurate phase (i.e., for large soliton density) the lines of constant $\eta$ can be found by a Kosterlitz-Thouless–type renormalization-group theory using the condition that scaling stops when the cutoff length becomes comparable to the distance between the solitons. Asymptotically, the value of $\eta$ for $\mu>>\mu_c$ is then simply given by the harmonic theory obtained by neglecting the cosine term in (1), i.e.,

$$\eta\rightarrow g/2\pi=\beta^2/2\pi p^2 \text{ as } \mu\rightarrow\infty\ . \quad (2)$$

Closer to the $CI$ transition, the soliton density becomes low, and the scaling trajectories diverge out of the range of validity of the simple Kosterlitz-Thouless theory. Here we must use the general Bethe-ansatz integral equations[8] for $\eta$. Close to the $CI$ transition, they simplify to give

$$\tfrac{1}{2}p^2\eta-1=4\sqrt{2}R(\beta)[\mu/\mu_c(\beta)-1]^{1/2}\ , \quad (3)$$

where $R(\beta)$ is a certain function of $\beta$.[14] As $\mu\rightarrow\mu_c$, we find $\eta\rightarrow 2/p^2$, which was first obtained by Schulz[15] in the present context (the equivalent result was independently obtained by Haldane[16] in the context of the $CI$ transition exhibited by the Heisenberg-Ising quantum spin chain).

The resulting curves of constant $\eta$ in the $\mu-T$ phase diagram are depicted in Fig. 2. The lines with $p^2\eta<2$ all flow to the point $T=0$, $\mu=\mu_c(0)$. For $0<T<T_{\max}$, $p^2\eta\rightarrow 2$ as $\mu\rightarrow\mu_c(T)$. As $T\rightarrow T_{\max}$,

$$\mu_c(T)\sim\mu_c(0)\exp(-\text{const}|T-T_{\max}|^{-1/2})\rightarrow 0\ ,$$

and for $2<p^2\eta<4$, the constant-$\eta$ lines flow to $T=T_{\max}$, $\mu=0$, as $c(\eta)\mu_c(T)$, where $c(\eta)$ increases monotonically from 1 to $\infty$ in this range. However, if $\mu\rightarrow 0$ at $T=T_{\max}$, $p^2\eta\rightarrow 4$, and the line $p^2\eta=4$ flows to $\mu=0$, $T=T_{\max}$, as $\text{const}[\mu_c(T)]^{1/2}$. For $p^2\eta>4$, the constant-$\eta$ lines hit the $\mu=0$ line at $T>T_{\max}$, doing so in a cusp for $p^2\eta<5$ but crossing the $\mu=0$ line smoothly (though with residual nonanalyticity) when $p^2\eta>5$.

We now apply the Kosterlitz-Thouless theory to determine the melting of the incommensurate phase by dislocation-pair unbinding. The philosophy we use is the same as that used by José *et al.*[3] when $\mu=0$, and by Villain and Bak[4] near $T=0$. When $\eta<\frac{1}{4}$ the $I$ phase is stable; when $\eta>\frac{1}{4}$ it is unstable with respect to dislocation unbinding and it melts. In the limit of weak vorticity $\eta$ is given by the value calculated in the absence of dislocations, i.e., the value we have already determined. *For a given value of p, the zero-vorticity limit of the melting line is the curve* $\eta=\frac{1}{4}$ *in Fig. 2.* This leads directly to the phase diagrams in Fig. 1 for $p=1$, 2, 3, 4, and 5. (For $p=1$ and $p=2$ the old $CI$ line is modified as discussed below, since dislocations are relevant.) At finite vorticity, renormalizations increase $\eta$ above $\eta$(zero vorticity) in the $I$ phase: This correction will be regular everywhere except in the vicinity of the line $\mu=0$.

The case $p=1$ is special since the liquid phase resulting from the dislocation-induced melting of the $I$ phase is indistinguishable from the $C$ phase with interstitials and vacancies. The commensurate "order parameter" is always nonzero since the periodic substrate potential acts as a field conjugate to it—just as for a ferromagnet in a magnetic field. The *CI* line is washed out and only an *IL* (or *IC*) line remains.[17] At zero temperature, this is a transition due to vanishing soliton density, but for $T>0$, it is a Kosterlitz-Thouless transition. Similar conclusions have been reached by Schaub and Mukamel.[18]

For $p=2$, the transition between $L$ and $C$ phases is an Ising transition (Bohr, Pokrovsky, and Talapov, Ref. 6). For one value of $T$, given by $\beta^2=4\pi$, their Hamiltonian could be diagonalized exactly, and there is no $I$ phase at this temperature. (We predict the $I$ phase to exist only at *lower* temperatures, $\beta^2\simeq 2\pi$.) Furthermore, in Ref. 6 it was found that dislocations lower the values of $\mu_c(T)$ and $\beta_{\max}$ as shown in Fig. 1 (full line) below the values given by the theory of the sine-Gordon model (1) [Fig. 1(b), dotted line].

For $p=3$ and $p=4$, our simple theory predicts that the melting and *CI* lines meet at the singular point $\mu=0$, $T=T_{\max}$, which by symmetry should be a $p$-state clock point. For $p=3$, this contradicts the common belief[10–16] that there should be a Lifshitz point at finite $\mu$ where the $L$, $C$, and $I$ phases meet, and thus a whole Potts (or Potts-type[12]) line for small $\mu$ near $T_{\max}$. The evidence for such a Lifshitz point comes from Monte Carlo simulations[11] and series expansions,[13] but does not seem conclusive.

Our method applies only for vanishing fugacity of dislocations, so the immediate vicinity of the Potts point really lies beyond our reach. At finite fugacity, it is possible that the Potts point might thus extend to a line in a small region around the symmetric ($\mu=0$) Potts point. On the other hand, Huse and Fisher[12] have analyzed the stability of the symmetric $p=3$ Potts point with respect to chirality $\mu$. Using scaling laws and the known Potts exponents, *they find that $\mu$ represents a relevant perturbation.* Our prediction of an isolated Potts point at $\mu=0$, with an $I$ phase separating the $C$ and $L$ phases at all finite $\mu$, would be a natural realization of this result.

We suggest further experiments and numerical calculations, in particular in the cases $p=1$ and $p=3$, in order to test our predictions. Since this work was completed, H. J. Schulz (private communication) has informed us that he has independently reached similar conclusions on the $p=3$ critical structure. He has also pointed out that, provided the positive crossover exponent for $\mu$ is smaller than 1, the cusps in Fig. 1 at points $P_3$ and $P_4$ are removed (as in the $p=2$ case).


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$$H=\sum_n (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \mu S_n^z + y S_n^x) \ .$$

Here $y$ describes the effects of dislocations, and corresponds to a magnetic field in the $x$-$y$ plane which destroys the $y=0$ phase transitions at $\mu=\pm 1$.

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