Commensurate-Incommensurate Transition in a Two Dimensional Classical Sine-Gordon System

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The critical line for the commensurate-incommensurate transition in the two dimensional classical sine-Gordon system is determined with the use of the Bethe ansatz equations for the massive Thirring model with finite hole density. Except slight differences the behavior of the critical line is the same as that obtained on the basis of the self-consistent harmonic phonon approximation.

Recently there has been much interest in the effect of thermal fluctuations on transitions between commensurate (C) and incommensurate (I) phases in two dimensional (2-D) systems. Especially sine-Gordon systems which exhibit the essence of the C-I transition are investigated in detail by many authors. The purpose of this letter is to discuss the C-I critical line for the 2-D classical sine-Gordon system with the use of the Bethe ansatz equations derived by Haldane for the massive Thirring model with finite hole density.

We start with the following 2-D classical sine-Gordon system:

\[ H = \sum_{\langle i,j \rangle} [J_x (h(i+1, j) - h(i, j) + \delta)^2]
+ f_x (h(i, j+1) - h(i, j))^2
- 2V \cos 2\pi h(i, j)] \tag{1} \]

where \((i, j)\) denote the lattice sites. In the language of physisorbed systems, \(h(i, j)\) is the displacement of the atom in one direction. The parameters \(J_x\), \(f_x\), and \(V\) are, respectively, the elastic constants and the strength of the substrate potential. The natural misfit \(\delta\) is the difference of the two characteristic lengths, namely, the natural distance between adatoms in the absence of the substrate potential and the period of the substrate potential.

Under the assumption that \(J_x \gg f_x \gg V\) we apply the transfer matrix technique\(^{14-15}\) for (1) and make the continuum approximation to obtain the 1-D quantum sine-Gordon system:

\[ H_{qs} = \frac{1}{2} \int dx \left[ p^2 + \left( \frac{\partial \phi_x}{\partial x} + \delta \right)^2 - \frac{2m_0}{g_\phi^2} \cos \phi \right] \tag{2} \]

where \(\delta = 2\pi \delta / gc\), \(\alpha_s = (2\pi)^2 V/J_x c^2\), \(g_s^2 = 2\pi^2 T/\sqrt{J_x f_s}\) with \(T\) and \(c\) being the temperature and the lattice constant of the original 2-D system.

The quantum Hamiltonian (2) may be transformed into a massive Thirring model (1-D interacting spinless fermion model)\(^{16,18}\) with the use of the boson representation of fermion fields.\(^{19}\) From this representation it follows that the misfit parameter in the sine-Gordon system corresponds to the chemical potential in the massive Thirring model:

\[ H_{mt} = \int dx \left[ v_F \left\{ -i \left( \phi_+^* \frac{\partial}{\partial x} \phi_+ - \phi_-^* \frac{\partial}{\partial x} \phi_- \right) \right.ight.
\left. \right. \left. - \delta \left( \phi_+^* \phi_+ + \phi_-^* \phi_- \right) \right] \]
\[ + m_0 \left( \phi_+^* \phi_+ + \phi_-^* \phi_- \right) \]
\[ + 2\phi_+^* \phi_+^* \phi_- \phi_-^* \tag{3} \]

where \(v_F = (4\pi / g_s^2 + g_s^2 / 4\pi) / 2 \approx 1\), \(\delta = g_\delta / 2\), \(m_0 = \alpha_s c / g_s^2 \approx \alpha_s c (1 - g_s^2 / 8\pi) / 2\pi\) (\(\alpha_s = e^{-\gamma_e} \approx 0.5772\): The Euler's constant),
and \( g_0 = (4\pi g^2 - g^4/4\pi) / 2 \approx \pi (1 - g^4/4\pi) \).

Here we have assumed the weak coupling limit \( g_0 \approx 0 \), i.e., \( g^2 \ll 4\pi \) and retained the lowest order term of interaction. The Fermi-Bose relations in solid state physics (with finite cutoff momentum) are only valid when \( m_0/v_f \) and \( g_0/v_f \) take small values so that the deep states of the Fermi sea are not so much altered by interactions.\(^{17}\)

We note that the relation between the misfit parameter \( \delta \) and the chemical potential \( \mu \) is different from that given by previous works,\(^{14,21,22}\) in which the zero momentum component \( (k = 0) \) in the boson fields was not treated carefully. In Haldane's paper\(^{20}\) we can see careful treatment of \( k = 0 \) component.

In the case \( g_0 = 0 \), the Hamiltonian is reduced to that of massive free fermion fields and is exactly diagonalized to allow the exact treatment for the C-I transition at particular temperature \( (T/\sqrt{J_1 J_2} = \pi/\pi) \) in the original 2-D classical sine-Gordon system.\(^{14,18,19}\) Our interest is in the C-I transition at general temperatures which correspond to the case \( g_0 \neq 0 \) in the massive Thirring model. The Hamiltonian of the massive Thirring model was diagonalized by formulating a Bethe ansatz.\(^{21,22}\)

Recently Haldane\(^{20}\) and Okwamoto\(^{23}\) have derived the renormalized Bethe ansatz equations which describe the ground state properties of the massive Thirring model with finite hole density. Using the results obtained in the massive Thirring model, they have discussed the C-I transition in the sine-Gordon system. On that occasion they have used the field theoretic correspondence\(^{24}\) between the sine-Gordon system and the massive Thirring model. The bare mass of the massive Thirring model has not been given explicitly in terms of \( J_1, J_2 \) and \( V \) of the original two dimensional problem.

Okwamoto has identified the renormalized mass in the massive Thirring model as the soliton formation energy which is obtained by means of the self-consistent harmonic phonon approximation in the sine-Gordon system. Therefore the C-I transition line has been the same as that obtained by Takayama.\(^{7}\) In this letter we will derive the C-I transition line in the context of the Hamiltonian of the massive Thirring model \( (3) \) without relying upon the result obtained in the sine-Gordon system.

In the following discussion we will assume the same rapidity cutoff in both the C- and I-state. This cutoff scheme in the Bethe ansatz equations is similar to that of Haldane but is different from that of Okwamoto, who has used the quantum number cutoff.

Putting the theory in a box of length \( L \) and imposing a periodic boundary conditions on the Bethe ansatz wave function for the massive Thirring model, we get\(^{21,22}\)

\[
m_0 \sinh \beta_i = -\frac{2\pi}{L} n_i - \frac{1}{L} \sum_j \phi(\beta_i - \beta_j), \quad (4\text{a})
\]

\[
\phi(\beta_i - \beta_j) = \frac{1}{L} \ln \left( \frac{-\sinh(\beta_i - 2\mu)}{\sinh(2\mu)} \right) \quad (4\text{b})
\]

and the eigenvalue

\[
E = \sum_i (m_0 \cosh \beta_i - \delta), \quad (5)
\]

where \( n_i \) are integers and rapidity variables \( \beta_i \) are introduced instead of quasi momentum \( k_i = (m_0 \sinh \beta_i) \). The parameter \( \mu \) is related to \( g_0 \) as \( \mu = -\cot^{-1}(g_0/2) \approx (\pi + g_0)/2 \). In the following discussion we restrict ourselves to the region \( \pi/3 < \mu < \pi \), where no strings appear in the ground state.\(^{23}\)

First we consider the filled Dirac sea which corresponds to the C-state. There are no holes in the vacuum modes and the distribution function \( \rho(\alpha) \) for rapidities \( \beta = i\pi + \alpha \) \( (\alpha: \text{real}) \) satisfies

\[
m_0 \cosh \alpha = 2\pi \rho(\alpha) + \int_{-\pi}^{\pi} da' \rho(\alpha') K(\alpha - \alpha'), \quad (6\text{a})
\]
Here a rapidity cutoff $\Lambda$ has been introduced. This equation can be solved in the limit $\Lambda \to \infty$, yielding\(^{21)}

$$\rho(a) = \frac{m_0}{2} \frac{\gamma - 1}{\sin 2\mu} \sinh \gamma a,$$

(7)

where $\gamma = \pi/2\mu$.

In a similar way we define the distribution function $\tilde{\rho}(a)$ in the $\Gamma$-state. In this case we assume holes in the interval $-\epsilon < a < \epsilon$ along the line $\beta = i\pi + a$ on the rapidity plane. Here we are thinking about the case $\delta < 0$. The distribution function satisfies

$$m_0 \cosh a = 2\pi \tilde{\rho}(a)$$

$$+ \left( \int_{-\epsilon}^{-\Lambda} \int_{\epsilon}^{\Lambda} da' \tilde{\rho}(a') K(a-a') \right).$$

(8)

The difference of the ground state energies $\Delta E = (E_\Gamma - E_\Sigma)$ and the fermion numbers $\Delta N = N_\Gamma - N_\Sigma$ between the $C$- and the $\Gamma$-state are, respectively, given by

$$\frac{\Delta E}{L} = - \left( \int_{-\epsilon}^{-\Lambda} \int_{\epsilon}^{\Lambda} m_0 \cos a \tilde{\rho}(a) da \right)$$

$$+ \int_{-\epsilon}^{-\Lambda} m_0 \cosh a \tilde{\rho}(a) da - \tilde{\delta} n,$$

(9-a)

$$\frac{\Delta N}{L} = n \left( \int_{-\epsilon}^{-\Lambda} \int_{\epsilon}^{\Lambda} \tilde{\rho}(a) da \right)$$

$$- \int_{-\epsilon}^{-\Lambda} m_0 \tilde{\rho}(a) da.$$  

(9-b)

Defining\(^{21)}$$ as $\Delta \rho(a) = \tilde{\rho}(a) - \rho(a)$ and subtracting (6-a) from (8), we get

$$0 = \Delta \rho(a) + \int_{-\epsilon}^{-\Lambda} da' \Delta \rho(a') K(a-a')$$

$$- \int_{-\epsilon}^{-\Lambda} da' \tilde{\rho}(a') K(a-a').$$  

(10)

This equation can be solved in the limit $\Lambda \to \infty$ via Fourier transformation and yield

$$\Delta \rho(a) = \frac{1}{2\pi} \int_{-\epsilon}^{\epsilon} da' \tilde{\rho}(a')$$

$$\times \left[ \hat{K}(y) \frac{dy}{2\pi} \right],$$

(11-a)

$$\hat{K}(y) = \int_{-\epsilon}^{\epsilon} K(a) e^{i\gamma a} \frac{dy}{2\pi}$$

$$= \frac{\sinh(\pi - 2\mu)y}{\sinh \pi y}.$$  

(11-b)

Putting (11-a) and (11-b) into (9-a) and (9-b), we finally obtain

$$\frac{\Delta E}{L} = 2\pi \int_{-\epsilon}^{\epsilon} \tilde{\rho}(a) \tilde{\delta} n,$$

(12-a)

$$n = \frac{1}{1 + \tilde{K}(0)} \int_{-\epsilon}^{\epsilon} \tilde{\rho}(a) da,$$

(12-b)

with the use of (12-b) and $\mu = (\pi + k_0)/2 = \pi (1 - g^2/8\pi)$.\(^{21)}

Making an expansion over $\epsilon$ in (12-a) and (12-b) and noting that $\rho(a) = \rho(a) + O(\epsilon)$, we obtain the following expression:

$$\frac{\Delta E}{L} = A n + B n^2,$$

(14)

where $A = -2\pi \tilde{\rho}(0)(1 + \tilde{K}(0)) - \tilde{\delta}$ and $B = -\pi^2(1 + \tilde{K}(0)^2)/(12\tilde{\rho}(0))$. From this expression we get the critical exponent $1/2$ for the C-I transition, which has been derived by Haldane and Villain\(^{21)}$$ and Okawamoto.\(^{21)}$$ The C-I transition line, which is obtained from $A = 0$, is written as

$$\delta_\epsilon = \frac{1}{4} \frac{g^2}{\sin(g\pi/4)} \left[ 1 - \frac{g^2}{8\pi} \right]$$

$$\times \left[ a_0 \left( 1 - \frac{g^2}{8\pi} \right) \frac{V}{J_a} + \rho^{(\phi)} \right],$$

(15)

in terms of original 2-D sine-Gordon system. Here we have assumed the relation $m_0 a = \sinh A$\(^{21)}$$ between the momentum cutoff $a$ and the rapidity cutoff $\Lambda$. We note that this

\(^{21)}$$ Putting $\mu = \pi (1 - g^2)/8\pi$, $n_0 = -(g^2/4\pi) n$, we get the relation $n_0 = -2(1 - \mu/\pi) n$, obtained by Hida, Imada and Ishikawa.\(^{21)}$$

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\(^{21)}$$ Downloaded from https://academic.oup.com/ptp/article-abstract/60/1/1291/1881499 by guest on 12 March 2019
equation (15) is only valid near $g^2=4\pi$. However the dependence of $\delta$ on $V/J_x$ is the same over the whole range of temperatures as that obtained in the self-consistent harmonic phonon approximation for the 1-D quantum sine-Gordon model. We have restricted our discussion to the case $\delta<0$. For the case $\delta>0$, from the symmetry of the original sine-Gordon system we may expect that the critical line is given by (15) except the difference of the sign. To treat the strong repulsive case ($0<\mu<\pi/3$) is left for a future study.

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