The Critical Properties of a Modulated Quantum Sine-Gordon Model

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(March 22, 2022)
Abstract

A new procedure of trial variational wave functional is proposed for investigating the mass renormailzation and the local structure of the ground state of a one-dimensional quantum sine-Gordon model with linear spatial modulation, whose ground state differs from that without modulation. The phase diagram obtained in parameters $(\alpha \Lambda^{-2}, \beta^2)$ plane shows that the vertical part of the boundary between soliton lattice phase and incommensurate (IC) phase with vanishing gap sticks at $\beta^2 = 4\pi$, the IC phase can only appear for $\beta^2 \geq 4\pi$ and the IC phase regime is enlarged with increasing spatial modulation in the case of definite parameter $\alpha \Lambda^{-2}$. The transition is of the continuous type on the vertical part of the boundary, while it is of the first order on the boundary for $\beta^2 > 4\pi$.

PACS: 05.70.Jk, 68.10.-m,87.22.Bt

Keywords: Sine-Gordon model, spatial modulation, soliton lattice, incommensurate phase, phase diagram

I. INTRODUCTION

Recently, many experiments have detected there exists a soliton lattice phase between spatially homogenous commensurate phase with finite gap and incommensurate (IC) phase with vanishing gap (free massless boson field) when some quasi-one-dimensional(1D) spin-Peierls (SP) materials were placed in an external magnetic field. These experiments confirm the 20-year-old prediction of a field-induced transition from the SP state into a spin-lattice modulated phase and demonstrated that this novel phase has the form of a soliton lattice. The density of solitons can be tuned continuously by adjusting the magnetic field, so that their internal structure can be systematically studied.

In deed, physical realization of SP systems offers the unique possibility to check the understanding of this fundamental 1D Hamiltonian for arbitrary band filling. Applying
the canonical Jordon-Wigner transformation, the Hamiltonian of such a SP chain placed in an external magnetic field $H$ can be mapped onto that of interacting (spinless) fermions system with band filling tuned by $H$. An convenient way to deal with 1D fermi systems is bosonization. After adopting the bosonization technique, the Hamiltonian of such a 1D fermi system is transformed into a modified sine-Gordon model with a linear spatial modulation in the cosine potential. In the boson picture, the effective Hamiltonian is

$$H = \int dx \left\{ \frac{1}{2} \left[ \Pi^2(x) + (\partial_x \phi)^2 \right] - \frac{\alpha}{\beta^2} \cos (\beta \phi + \lambda x) \right\}. \quad (1)$$

Here $\phi(x)$ is a boson field operator, $\Pi(x)$ is its conjugate momentum, $\Pi(x) = -i \delta \phi(x)$, and they satisfy the commutation relation

$$[\phi(x), \Pi(y)] = i \delta(x - y). \quad (2)$$

$\lambda$ is a spatial modulation parameter, which represents the effect of fermi surface shifting from half filling in the fermion picture.

Although the Zeeman energy influences the comparison between the ground state energy of boson models with different modulation, it has no effect to the structure of the ground state for fixed band filling case. It is neglected in present paper.

An alternative realization of the Hamiltonian (1) with fixed $\lambda$ refers to the interaction fermion system with tunable particle concentration. For example, the charge-density-wave degree freedom of the 1D extended Hubbard model is described by this model. Away from the half filling, or $\lambda \neq 0$, people usually assumes that the cosine potential can be neglected due to the rapid oscillation. However, according to this statement, the energy gap would drop suddenly to zero at $\lambda = 0$. We believe it is more likely that the cosine potential might experience an intermediate lattice phase before entering into the free boson field regime.

In absence of $\lambda$, the Hamiltonian is a standard quantum sine-Gordon model. Many works have been done about this case both in field theory and in condensed matter physics. By a variational method Coleman first discovered that the energy density of the system
is unbounded below when the coupling constant $\beta^2$ exceeds $8\pi$, this corresponds to the Kosterlitz-Thouless (K-T) phase transition by the equivalence between the 2D Coulomb gas and sine-Gordon model, the ground state is a spatially homogenous commensurate phase.

In presence of finite $\lambda$, the spatial modulation parameter favors the IC phase whereas the cosine term itself favors the commensurate phase, this makes the model more complicated. Previously, many results for the Hamiltonian (1) have been obtained in the classical limit. [17–19] In the quantum case, this cosine potential is usually considered to shrink to zero with any finite $\lambda$, the crossover between commensurate and IC phases would happen abruptly. Schulz has discussed a similar quantum system as Hamiltonian (1) [20], he found that the domain wall structure appeared in the ground state in the case of the chemical potential exceeding a threshold value and the energy gap was finite, for large chemical potential the presence of the gap was unimportant. In fact, his result implied that there existed a soliton lattice phase which had finite density of domain walls between commensurate phase with finite gap and IC phase with vanishing gap.

After taking a shift $\phi(x) + \frac{\lambda x}{\beta} \rightarrow \phi(x)$, the Hamiltonian (1) seems as same as that of Schulz. But if one pays attention to the boundary condition of boson operator $\phi(x)$, he will find that two models are different since the boundary conditions of system will be altered under this shift, namely, $\int_0^{L} \partial_x \phi(x) dx = 0 \rightarrow \int_0^{L} \partial_x \phi(x) dx = \frac{\lambda}{\beta}L$, therefore the physical properties will be also changed. We prefer the former (zero charge sector), since this integral is proportional to the particle number after normal ordering in the fermion picture. To our knowledge, with finite $\lambda$, the complicated configuration between commensurate and IC phases has not been explored clearly.

In present paper, we develop a new method to give a quantitative discussion on the soliton lattice phase of the Hamiltonian (1). Our basic idea refers to a variational procedure with respect to a spatially inhomogenous Gaussian wave functional which is introduced to determine an approximate ground state of the model. Our results show that as long as $\lambda$ shifts from zero, the soliton lattice phase appears in the ground state for $\beta^2 < 4\pi$. Only in the regime of $\beta^2 > 4\pi$ the IC phase with vanishing gap can emerge in the ground state.
for small $\alpha$. The paper is set up as following. In section II, we introduce a new spatially inhomogenous Gaussian wave functional and calculate the energy and the renormalization mass of the ground state. The phase diagram and the evolvement of the soliton lattice phase with varying spatial modulation parameter are given in section III. Section IV is our conclusion.

**II. SPATIALLY INHOMOGENIOUS GAUSSIAN WAVE FUNCTIONAL METHOD**

In the Schrodinger field picture, the problem is to solve the functional Schrodinger equation

$$H\Psi = E\Psi$$

where $\Psi$ is a wave functional of the variable $\phi(x)$. It is obviously difficult and far beyond our present abilities to solve this equation for the Hamiltonian (1). Here we try a variational method by choosing some general ansatz for $\Psi$, then we calculate the expectation value of the Hamiltonian and minimize the energy with respect to the variational parameters in the ansatz.

If we consider the field operator $\phi(x) = 0$, the cosine term will oscillate in the space yielding zero contribution to the ground state. This may not be the most favorable configuration of the ground states. One may shift $\phi(x)$ to compensate $\lambda x$ as much as possible to lower the value of the cosine potential term, however, the integration of $\partial_x \phi$ should be zero since it must satisfy the boundary condition. Thus $\phi(x)$ should take a kink after some distance, moreover, the modulation of $\phi(x)$ induces a ”distortion energy” $\frac{1}{2}(\partial_x \phi)^2$. Nevertheless, we expect an appropriate form of $\phi(x)$ which can lower the total energy at most.

Taking above into consideration, we approach the ground state of the system by a trial Gaussian wave functional with a field shift as
\( \Psi(P, \phi_{cl}, f) = N_f \exp \left \{ i \int P(x) \phi(x) dx - \frac{1}{2} \int dxdy \left [ (\phi(x) - \phi_{cl}(x)) f(x, y) (\phi(y) - \phi_{cl}(y)) \right ] \right \}. \) (4)

Where \( N_f \) is the normalization factor, \( P(x), \phi_{cl}(x) \) and \( f(x, y) \) are the variational functions. The expectation value of the Hamiltonian of Eq.(1) with respect to the wave functional of Eq.(4) is given in as

\[
E(P, \phi_{cl}, f) = \int dx \left \{ \frac{1}{2} \left [ P(x)^2 + (\partial_x \phi_{cl}(x))^2 \right ] - \frac{\alpha}{\beta^2} Z \cos (\beta \phi_{cl}(x) + \lambda x) \\
+ \frac{1}{4} f(x, x) - \frac{1}{4} \int dy \delta(x - y) \frac{\partial^2}{\partial_x \partial_y} f^{-1}(x, y) \right \},
\]

(5)

where

\[
Z = \exp \left \{ -\frac{\beta^2}{4} f^{-1}(x, x) \right \}, \quad (6)
\]

\( f^{-1}(x, y) \) denotes the inverse of \( f(x, y) \), i.e.,

\[
\int f(x, x') f^{-1}(x', y) dx' = \delta(x - y).
\]

For simplicity we choose \( f(x, y) \) of the form

\[
f(x, y) = \frac{1}{2\pi} \int dk \sqrt{k^2 + \mu^2} \cos k(x - y)
\]

with inverse

\[
f^{-1}(x, y) = \frac{1}{2\pi} \int dk \frac{\cos k(x - y)}{\sqrt{k^2 + \mu^2}}, \quad (7)
\]

where \( \mu^2 \) is a variational parameter.

Up to now, we have introduced three variational parameters \( P(x), \phi_{cl}(x) \) and \( \mu^2 \) which will be determined in the following calculation. For the ground state, the minimal energy configuration is clearly achieved with \( P(x) = 0 \).

Introducing a upper cutoff \( \Lambda \) in the integral of Eq.(7), Eq.(6) is explicitly evaluated as

\[
Z = \left ( \frac{\mu \Lambda^{-1}}{1 + \sqrt{1 + (\mu \Lambda^{-1})^2}} \right )^{\frac{\beta^2}{4\pi}}, \quad (8)
\]

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and the expectation energy is
\[
E(\phi_{cl}, \mu^2) = \int dx \left\{ \frac{\Lambda^2 \sqrt{1 + (\mu \Lambda^{-1})^2}}{4\pi} + \frac{1}{2} \left( \partial_x \phi_{cl}(x) \right)^2 - \frac{\alpha}{\beta^2} Z \cos (\beta \phi_{cl}(x) + \lambda x) \right\} \quad (9)
\]

After minimizing the energy expectation value with respect to \(\mu\) and \(\phi_{cl}(x)\) respectively, we get
\[
\mu^2 = \alpha Z \frac{1}{L} \int dx \cos \theta(x),
\]
\[
\frac{\partial^2 \theta(x)}{\partial x^2} = \alpha Z \sin \theta(x). \quad (10)
\]
Here, we have set \(\theta(x) = \beta \phi_{cl}(x) + \lambda x\) for brevity, \(L\) is the macroscopic length of the system.

Eq.(10) is a soliton equation, integrating the above equation with variation of \(\theta(x)\), we get
\[
\frac{d\theta}{dx} = \pm \sqrt{2\alpha Z (c - \cos \theta)} \quad (11)
\]
where \(c\) is a integration constant and it satisfies
\[
\frac{2\sqrt{2}}{\sqrt{c+1}} K \left( \frac{\sqrt{2}}{\sqrt{c+1}} \right) = \frac{2\pi \sqrt{\alpha Z}}{\lambda} \quad (12)
\]
according to the boundary condition \(\int_0^L \partial_x \phi dx = 0\). Here \(K \left( \frac{\sqrt{2}}{\sqrt{c+1}} \right)\) is the first class elliptical integral function. The renormalization mass equation is simplified as
\[
\mu^2 = \alpha Z \left[ \frac{2\sqrt{2} c}{\sqrt{c+1}} K \left( \frac{2}{\sqrt{c+1}} \right) - 2\sqrt{2 (c+1)} E \left( \frac{2}{\sqrt{c+1}} \right) \right]. \quad (13)
\]

\(E \left( \frac{2}{\sqrt{c+1}} \right)\) is the second class elliptical integral function. The approximate energy density of the ground state is
\[
\varepsilon_0(\lambda) = \frac{\Lambda^2 \sqrt{1 + (\mu \Lambda^{-1})^2}}{4\pi} + \frac{1}{\beta^2} \left[ \alpha Z c - 2\mu^2 - \frac{1}{2} \lambda^2 \right]. \quad (14)
\]

**III. PHASE DIAGRAM AND SOLITON EVOLVEMENT OF THE GROUND STATE**

Since Eq.(11) involves elliptical function, it is difficult to be solved explicitly. Before solving it we give some analytic discussion at special conditions for \(c = 1\) or \(\infty\).
A. Two special cases

i) When \( c = 1 \), we know \( \lambda \Lambda - 1 = 0 \). The non-trivial solution of Eq.(11) represents one soliton,

\[
\cos 2\theta = \pm \tanh \sqrt{\alpha Z x}.
\]

For this case Nakano and Fukuyama have given a detailed discussion. What we should note is the modification of excitation gap near this case. After expanding the elliptical functions to linear terms of \( \lambda \Lambda - 1 \), we get an expression of the renormalization mass \( \mu \) as

\[
(\mu \Lambda^{-1})^2 = (\mu_0 \Lambda^{-1})^2 - \frac{2\lambda \mu_0 \Lambda^{-2}}{\pi}.
\]  

(15)

\( \mu_0 \Lambda^{-1} \) is the renormalization mass with \( \lambda \Lambda^{-1} = 0 \), it satisfies

\[
(\mu_0 \Lambda^{-1})^2 = \alpha \Lambda^{-2} \left( \frac{\mu_0 \Lambda^{-1}}{1 + \sqrt{1 + (\mu_0 \Lambda^{-1})^2}} \right)^{\frac{\beta^2}{4\pi}}.
\]  

(16)

If \( \beta^2 < 8\pi \), the above equation has a non-trivial solution with nonzero value of \( \mu_0 \Lambda^{-1} \). Eq.(15) implies that the excitation gap will trail off when \( \lambda \Lambda^{-1} \) shifts from zero. It should be noted that the ground state at finite \( \lambda \Lambda^{-1} \), whatever small, differs from the ground state at \( \lambda \Lambda^{-1} = 0 \), since the ground state is spatially inhomogenous with soliton lattice structure in the first case, whereas it is spatially homogenous commensurate phase in the second condition.

ii) When \( c \to \infty \), we get

\[
\frac{1}{L} \int dx \cos \theta(x) = \frac{\alpha \Lambda^{-2} Z}{2(\lambda \Lambda^{-1})^2},
\]  

so the renormalization mass equation is simplified as

\[
(\mu \Lambda^{-1})^2 = \left( \frac{\alpha \Lambda^{-2}}{\sqrt{2\lambda \Lambda^{-1}}} \right)^2 \left( \frac{\mu \Lambda^{-1}}{1 + \sqrt{1 + (\mu \Lambda^{-1})^2}} \right)^{\frac{\beta^2}{4\pi}}.
\]  

(18)

In the case of \( \beta^2 < 4\pi \), Eq.(18) always has a nonzero solution for the renormalization mass \( \mu \Lambda^{-1} \). When \( \beta^2 > 4\pi \), existence of a nonzero solution depends on the competition
between $\alpha \Lambda^{-2}$ and $\lambda \Lambda^{-1}$. In the special case of $\beta^2 = 4\pi$, it has only zero solution when $\alpha \Lambda^{-2} < 2\sqrt{2}\lambda \Lambda^{-1}$, while it has nonzero solution when $\alpha \Lambda^{-2} > 2\sqrt{2}\lambda \Lambda^{-1}$. For this special case the model can be solved exactly by mapping it into a modified Thirring model, which predicts similar result that the finite mass appears for sufficiently large $\alpha \Lambda^{-2}$.

**B. The phase diagram of the model**

In order to give an understandable phase diagram, we numerically solve the renormalization mass equation and soliton equation for a pair of parameters $(\alpha \Lambda^{-2}, \beta^2)$. The families of curves with constant renormalization masses for different values of $\lambda \Lambda^{-1}$ are depicted in the parameter plane, see Fig.1.

With any finite $\lambda \Lambda^{-1}$, we find that the ground state is always in the soliton lattice phase with finite renormalization mass in the range of $\beta^2 < 4\pi$. The IC phase with vanishing gap only appears in the range of $\beta^2 > 4\pi$, increasing of $\lambda \Lambda^{-1}$ leads to enlarging of IC phase area. It is clear that the transition is a continuous transition on the vertical line $\beta^2_c = 4\pi$ for $\alpha \Lambda^{-2} < 2\sqrt{2}\lambda \Lambda^{-1}$ since the renormalization mass tends to zero from the left side of it. The soliton lattice phase with finite renormalization mass is allowed in the range of $\beta^2 > 4\pi$. The phase diagram is shown in Fig.2 where the transition boundary consists of the envelope of the family $\mu \Lambda^{-1} =$constant with different values of $\lambda \Lambda^{-1}$. Under the boundary the renormalization mass vanishes, where the Hamiltonian (1) reduces to that of a free massless boson field, whereas upon the boundary the renormalization mass is nonzero. The first order transition occurs along this boundary in the range of $\beta^2 > 4\pi$.

In the area where the renormalization mass is finite, a soliton lattice phase emerges in the real space in the ground state. The local structure of the ground state are shown in Fig.3. It can be seen that the amplitudes of the oscillating part of the local solitons become smaller and the periods become shorter with increasing $\lambda \Lambda^{-1}$. In the soliton lattice phase, the real space in the ground state will split into many periodic domains $\frac{2\pi (n-1)}{\lambda} < x < \frac{2\pi (n+1)}{\lambda}$ ($n$ integer). In the area where the renormalization mass is zero, the amplitude of solitons
reduces to zero, the soliton lattice phase disappears, the ground state enters into a free boson regime.

IV. CONCLUSION

In this paper we have studied the behavior of the ground state of a sine-Gordon model with linear spatial modulation. The main task is to calculate the ground state and low excitations for constant modulation parameter. We have applied a variational procedure with respect to a Gaussian wave functional to find an approximate ground state. Our result shows that for $\beta^2 > 4\pi$ IC phase grows with increasing $\lambda$, where the low energy physics can be described by a free massless boson field theory, while upon the boundary the excitation gap is still finite, and the real space is no more homogeneous, a soliton lattice state appears. On the other hand, for $\beta^2 < 4\pi$, only the soliton lattice phase can exist. With increasing spatial modulation parameter, the soliton periodic length decreases, while the correlation length (inverse of the gap) increases. The transition type between soliton lattice phase and IC phase maybe of the continuous or first order, which relies on the varying of parameter $\beta^2$.

Applying above conclusion to the CDW degree freedom of the 1D extended Hubbard model whose parameter $\beta^2 = 8\pi \sqrt{\frac{2\pi t - 2V}{2\pi t + U + 5V}}$, we find the following assertion. The ground state is always in the soliton lattice phase in the case of $U + 13V > 6\pi t$, the umklapp term can not be neglected for any filling case. On the other hand when $U + 13V < 6\pi t$ the ground state maybe tuned to a free massless boson state when the band filling shifts away half filling sufficiently, only in this case the umklapp term can be directly cancelled.
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**Captions**

FIG.1 The families of curves with constant renormalization masses in the parameter $\alpha \Lambda^{-2} - \beta^2$ plane with (a) $\lambda \Lambda^{-1} = 10^{-6}$ , (b) $\lambda \Lambda^{-1} = 10^{-3}$ and (c) $\lambda \Lambda^{-1} = 10^{-1}$. The renormalization mass is chosen as $\mu_1 \Lambda^{-1} = 1$, $\mu_2 \Lambda^{-1} = 10^{-1}$, $\mu_3 \Lambda^{-1} = 10^{-3}$, $\mu_4 \Lambda^{-1} = 10^{-5}$, $\mu_5 \Lambda^{-1} = 10^{-7}$, $\mu_6 \Lambda^{-1} = 10^{-9}$ and $\mu_7 \Lambda^{-1} = 10^{-11}$.

FIG.2 Phase diagram of the model in the parameter $\alpha \Lambda^{-2} - \beta^2$ plane with different values of $\lambda \Lambda^{-1}$. The regions I and II represent soliton lattice phase and IC phase respectively.

FIG.3 The local forms of the soliton lattice phase for $\lambda \Lambda^{-1} = 0.004$ (a) and $\lambda \Lambda^{-1} = 0.01$ with $\alpha \Lambda^{-2} = 0.2$ and $\beta^2 = 5\pi$. Here, we take $\frac{\partial \theta(x)}{\partial x}$ as function of coordinate $x$, since it is proportional to the effective cosine potential.
Fig. 1 (b) \( \lambda \Lambda^{-1} = 10^{-3} \) vs. \( \beta^2 / 8\pi \)
Fig. 1 (c) $\lambda \Lambda^{-1} = 10^{-1}$

$\alpha/\Lambda^2$ vs $\beta^2/8\pi^1$

- $\mu \Lambda^{-1} = 3$
- $\mu_1$
- $\mu_2$
- $\mu_3$
- $\mu_4$
- $\mu_5$
- $\mu_6$
- $\mu_7$
Fig. 1 (a) \( \lambda \Lambda^{-1} = 10^{-6} \)
Fig. 2 (a) $\lambda \Lambda^{-1} = 10^{-6}$
Fig. 2 (b) $\lambda \Lambda^{-1} = 10^{-3}$
Fig. 2 (c) $\lambda \Lambda^{-1} = 10^{-1}$
$d\theta(x)/dx$

Fig. 3