Bound state in a one-dimensional quantum sine-Gordon model

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The impurity problem in a one-dimensional quantum sine-Gordon model is studied in this paper. We use an analytic self-consistent theory to derive the excitation spectrum of the global sine-Gordon model, and then to study the bound state induced by local impurity. We give the conditions where an impurity level exists within the global gap of the excitation spectrum and show the possibility of the existence of a threshold value about the model parameter. [S0163-1829(98)03703-5]

Doping effects on one-dimensional spin chains have attracted great interest in recent years. For example, experimental and theoretical studies indicate that doping strongly affects the transition temperature and magnetic energy gap in the spin-Peierls compound $CuGeO_3$.[1,2] As another example, the bound state due to off-chain impurity in an $S=1$ Heisenberg spin chain has recently been studied theoretically by some authors.[3–5] In Ref. 3 the Schwinger-boson approach is used to find that when the bond-coupling deviation exceeds a threshold there exists a bound state and the impurity level is always located in the middle of the Haldane gap. Other issues exist in Refs. 4 and 5. In both of them the numerical density-matrix renormalization-group method is used and the conclusion that the impurity energy level changes gradually as the strength of impurity bond changes is reported. Some concrete computational results, such as the value of threshold, etc., are given in both of them, however, the results do not absolutely coincide. So there still exist some unclear points about doping behavior in the spin system.

On the other hand, it is well known that the spin-Peierls system and the $S=1$ Heisenberg spin chain can all be mapped onto a one-dimensional (1D) sine-Gordon (SG) model via Jordan-Wigner transformation and bosonization.[6,7] Therefore, it is quite interesting to discuss the doping effects on these systems in the frame of SG model. Moreover, the SG model can also describe many other one-dimensional systems, such as the 1D Luttinger liquid,[8] the 1D Kondo array model,[9] etc. Recently numerical work regarding impurity in a Luttinger liquid has been reported.[10] Hence, the impurity problem in the SG model becomes a very important and very *universal* problem. In this paper we plan to study the single impurity problem in the SG model analytically. We try to give some general conclusions and we believe these results can be applied to various concrete models directly or after generalization.

Because of the difficulty of infrared divergence, the SG model itself is difficult to handle. The traditional perturbation approach becomes invalid due to strong correlation. The renormalization-group (RG) theory can give scaling flow of the model, however, it is difficult for it to give much other useful information, such as excitation spectrum, etc. Recently a quantum self-consistent theory[11] was developed to discuss the SG model. With it the infrared divergence is effectively treated and the energy gap in the spectrum can be obtained self-consistently. Here this method is used to treat SG model as a first step. Then the method is extended to treating the impurity problem in the SG model and the conditions for an impurity level within the gap are derived.

We start with the following Hamiltonian:

$$H=H_0+H_{\mathrm{imp}},$$

$$H_0=\int dx\{[\Pi^2+(\nabla\phi)^2]/2 - (\alpha_0/\epsilon^2\beta_0^2)\cos[\beta_0\phi(x)]\}, \tag{1}$$

$$H_{\mathrm{imp}}=-(\alpha_1/\epsilon\beta_0^2)\cos[\beta_0\phi(0)]-\alpha_2\epsilon\Pi^2(0).$$

Here H_0 is the usual global SG model Hamiltonian. H_{imp} contains two terms, representing the impurity interaction. The first term in H_{imp} describes the large momemtum transfer scattering, while the other describes small momentum transfer. Indeed, these two terms affect only the even parity components of the field $\phi(x)$ and they do not break the reflection symmetry. The term $f(\nabla\phi(0))$, which affects the odd parity components and breaks the reflection symmetry, is not considered in this paper, since we assume that the impurity is symmetric with respect to the origin $x=0$ and the model will keep invariance under the reflection transformation. ϵ is a short-distance (ultraviolet) cutoff and the whole model parameters $\alpha_0,\alpha_1,\alpha_2,\beta_0$ are dimensionless constants, of which α_0,β_0 are assumed positive. As a first step we treat the global SG term H_0. Here we briefly outline the procedures of self-consistent theory. In momentum space we first consider the following Bogoliubov transformation in order to treat infrared divergence:

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$$U=\exp\left[-\sum_k (\gamma_k/2)(b_k^\dagger b_{-k}^\dagger - b_k b_{-k})\right], \tag{2}$$

where γ_k is given by self-consistent results below and $b_k, b_k^\dagger$ satisfies the standard boson commutator. As pointed out in Ref. 12, the transformation (2) describes the real coordinates' amplification or reduction, similar to the idea of scaling change in RG theory. Secondly we normally order the cosine term in H_0 and expand it:

$$\begin{aligned}\tilde{H}_0 &= UH_0U^\dagger \\ &= \sum_k \{|k|\cosh 2\gamma_k + [\alpha\exp(-2\gamma_k)/(2\epsilon^2|k|)]\} b_k^\dagger b_k \\ &\quad + \left[\sum_k |k|(\cosh 2\gamma_k)/2 - \alpha/\epsilon^2\beta_0^2\right] \\ &\quad - \sum_k \{|k|\sinh 2\gamma_k - [\alpha\exp(-2\gamma_k)/(2\epsilon^2|k|)]\} \\ &\quad \times (b_k^\dagger b_{-k}^\dagger + b_k b_{-k})/2,\end{aligned} \tag{3}$$

where

$$\alpha \equiv \alpha_0\xi = \alpha_0\exp\left[-\left(\frac{\beta_0^2}{4}\right)\sum_k \exp(-2\gamma_k)/|k|\right]. \tag{4}$$

The terms higher than quadratic are omitted in Eq. (3). Thirdly we select appropriate γ_k in order to remove the nondiagonal term and give the following expression of γ_k:

$$\gamma_k = (1/4)\ln[1+(\alpha/\epsilon^2 k^2)]. \tag{5}$$

Now $\tilde{H}_0$ becomes a free field:

$$\tilde{H}_0 = \sum_k \omega_k b_k^\dagger b_k. \tag{6}$$

ω_k is the elementary excitation spectrum and written as $\omega_k = \sqrt{k^2+M^2}$. M is the global excitation gap or mass: $M = (\alpha_0\xi)^{1/2}/\epsilon$, ξ is given self-consistently as follows:

$$\xi = \exp\left[\frac{\beta_0^2/8\pi}{(\beta_0^2/8\pi)-1}\ln(\sqrt{\xi+\alpha_0^{-1}}+\sqrt{\alpha_0^{-1}})^2\right]. \tag{7}$$

From Eq. (7) we can see obviously that when $\beta_0^2 < 8\pi$, one nonzero solution of ξ can always be obtained, which means the SG model has finite energy gap. When $\xi \neq 0$, we find the higher-order terms that we have omitted in Eq. (3) are infrared convergent, which means the *self-consistency* of our theory. In the following we will study the impurity behavior based on $\tilde{H}_0$.

There are two terms relating to $H_{\rm imp}$. The second term is quadratic and easy to handle, so we lay it aside firstly and just consider the first term. After transformation (2) the first term in $H_{\rm imp}$ becomes

$$\begin{aligned}\tilde{H}_{\rm imp,1} &= U\left[-\frac{\alpha_1}{\epsilon\beta_0^2}\cos[\beta_0\phi(0)]\right]U^\dagger \\ &= -\frac{\alpha_1}{\epsilon\beta_0^2}\cos\left[\beta_0\sum_k \frac{1}{\sqrt{2L}}\frac{1}{\sqrt{\omega_k}}(b_k+b_k^\dagger)\right].\end{aligned} \tag{8}$$

Normal ordering the above term and collecting the quadratic terms together we obtain

$$\begin{aligned}\tilde{H}_{\rm imp,1} &= \frac{\alpha_1'}{\epsilon}\sum_{kk'} (2L\omega_k)^{-1/2}(2L\omega_{k'})^{-1/2} \\ &\quad \times [(b_k b_{k'} + b_k^\dagger b_{k'}^\dagger)/2 + b_k^\dagger b_{k'}],\end{aligned} \tag{9}$$

where

$$\begin{aligned}\alpha_1' &= \alpha_1 W, \\ W &= \exp\{-(\beta_0^2/2)\Sigma_k(1/2L\omega_k)\} \\ &= [(1+\sqrt{\alpha_0\xi+1})/\sqrt{\alpha_0\xi}]^{-\beta_0^2/4\pi}.\end{aligned}$$

In Eq. (9) the higher-order terms are omitted, just as we have done before. Here we have extended the self-consistent theory to the case where the local term is included. After these treatments the total Hamiltonian becomes quadratic and we can cope with it conveniently. The total Hamiltonian becomes (omitting constants)

$$\begin{aligned}\tilde{H} &= \tilde{H}_0 + \tilde{H}_{\rm imp}, \\ \tilde{H}_{\rm imp} &= \sum_{kk'}\left[\alpha_1'(2\epsilon)^{-1}(2L\omega_k)^{-1/2}(2L\omega_{k'})^{-1/2}\right. \\ &\quad \left. + \alpha_2\epsilon\left(\frac{\omega_k}{2L}\right)^{1/2}\left(\frac{\omega_{k'}}{2L}\right)^{1/2}\right](b_k b_{k'} + b_k^\dagger b_{k'}^\dagger) \\ &\quad + \sum_{kk'}\left[\alpha_1'\epsilon^{-1}(2L\omega_k)^{-1/2}(2L\omega_{k'})^{-1/2}\right. \\ &\quad \left. - 2\alpha_2\epsilon\left(\frac{\omega_k}{2L}\right)^{1/2}\left(\frac{\omega_{k'}}{2L}\right)^{1/2}\right] b_k^\dagger b_{k'},\end{aligned} \tag{10}$$

where $\tilde{H}_0$ is given by Eq. (6). In principle, the Hamiltonian $\tilde{H}$ can be diagonalized. To avoid searching for the complicated unitary transformation, we try to transform the creation and annihilation operators into canonical coordinates and momenta directly. Through constructing the equations of motion for canonical coordinates we can obtain the energy spectrum of Hamiltonian $\tilde{H}$, which is just what we want in this paper. Transforming the creation and annihilation operators into complex canonical coordinate and momentum Q_k and P_k:

$$b_k = \sqrt{\frac{\omega_k}{2}}\left(Q_k + i\frac{P_{-k}}{\omega_k}\right), \quad b_k^\dagger = \sqrt{\frac{\omega_k}{2}}\left(Q_{-k} - i\frac{P_k}{\omega_k}\right), \tag{11}$$

we can obtain the following equations of motion:

$$\ddot{Q}_k = -\omega_k^2 Q_k + \left(\frac{2\alpha_2}{\pi} - 1\right)\frac{\alpha_1'}{L\epsilon}\sum_{k'} Q_{k'} + \frac{2\epsilon\alpha_2}{L}\sum_{k'} \omega_{k'}^2 Q_{k'}. \tag{12}$$

Obviously the solution of Q_k has the form of $e^{i\omega t}$, ω is just the energy spectrum of $\tilde{H}$. Noting that wave vector k takes values $0, \pm 2\pi/L, \pm 4\pi/L, \ldots$ when the periodic boundary condition is assumed, we finally obtain the equation that ω must satisfy:

$$\left(\frac{2\alpha_2}{\pi}-1\right)\frac{\alpha_1'}{L\epsilon}f_1(\omega)+\frac{2\alpha_2\epsilon}{L}f_2(\omega)=1 \tag{13}$$

including the following definition:

$$f_1(\omega)=\sum_k \frac{1}{\omega_k^2-\omega^2}, \quad f_2(\omega)=\sum_k \frac{\omega_k^2}{\omega_k^2-\omega^2}.$$

As for Eq. (13) there may exist two kinds of solutions: the single solution $\omega<M$ and a series of solutions $\omega>M$. The single solution $\omega<M$ represents an impurity level within the gap of the SG model, which is just what we search for. When ω is constricted in the region $\omega<M$, the functions $f_1(\omega), f_2(\omega)$ are continuous for large L, so we can change the summation in $f_1(\omega)$ and $f_2(\omega)$ into the integral and obtain

$$f_1(\omega)=\frac{L}{2}(M^2-\omega^2)^{-1/2}$$

$$f_2(\omega)=\frac{L}{\pi}\left[\epsilon^{-1}+\frac{\pi}{2}\omega^2(M^2-\omega^2)^{-1/2}\right].$$

In the following we divide three cases to discuss in what conditions there exists the solution $\omega<M$. Before going on, we note the following fact: in our theory treating the global and local cosine term we just retain the quadratic terms and omit the higher-order terms after normal ordering. In Ref. 12 we have pointed out the results are satisfactory in the region $\alpha_0<1$ when the self-consistent theory is used to treat the usual global SG model. So in the following discussions we will restrict the model parameters in the relatively small regions, in which we think our theory is valid. Two dimensionless parameters are introduced: $\tilde{M}=M\epsilon, \tilde{\omega}=\omega\epsilon$, of which $\tilde{M}=(\alpha_0\xi)^{1/2}$ is usually less than 1 when $\alpha_0<1$.

(1) $\alpha_2=0, \alpha_1\neq 0$, Eq. (13) is simplified into

$$\alpha_1'=-2(\tilde{M}^2-\tilde{\omega}^2)^{1/2}=F_1(\tilde{\omega}). \tag{14}$$

Graphic solution is shown in Fig. 1, where the bound-state energy $\tilde{\omega}^*$ is determined by the intersection between the curves $F(\tilde{\omega})=F_1(\tilde{\omega})$ and $F(\tilde{\omega})=\alpha_1'$. We find the condition in which the solution $\omega<M$ exists is $\alpha_1<0$ (notice $W>0$).

(2) $\alpha_1=0, \alpha_2\neq 0$, Eq. (13) is simplified into

$$\alpha_2=\frac{\pi}{2}\left[1+\frac{\pi}{2}\tilde{\omega}^2(\tilde{M}^2-\tilde{\omega}^2)^{-1/2}\right]^{-1}=F_2(\tilde{\omega}). \tag{15}$$

Graphic solution is shown in Fig. 2. Similar to Eq. (1) we find the condition in which the solution $\omega<M$ exists is $\alpha_2>0$.

(3) General case: $\alpha_1\neq 0, \alpha_2\neq 0$, though $f_1(\omega), f_2(\omega)$ are all monotonously increasing functions, the left-hand side of Eq. (13) may not be monotonous. There exists competition between two parameters α_1 and α_2 in order to take on the solution $\omega<M$. We give the results in Fig. 3. There is only a shaded region where the solution $\omega<M$ exists. In the relatively small parameter region as shown in Fig. 3, the shaded region is decided by the condition

$$\alpha_1'<\frac{2\pi\alpha_2\tilde{M}^2}{\pi-2\alpha_2}.$$

The above results can be understood physically in the following description. In fact, roughly speaking, our treatment in this paper is equivalent to substituting the beginning Hamiltonian by

$$H_e=\int dx\{[\Pi^2+(\nabla\phi)^2]/2+M^2\phi^2(x)/2\}+c_1\phi^2(0)+c_2\Pi^2(0), \tag{16}$$

where the coefficients c_1, c_2 are proportional to $\alpha_1, -\alpha_2$ respectively. From the view of quantum mechanics, the terms $c_1\phi^2(0)$ and $c_2\Pi^2(0)$ can respectively give rise to a δ potential barrier or well, decided by the sign of $c_1(c_2)$. Here it must be noted that only *in the case of a well can there exist*

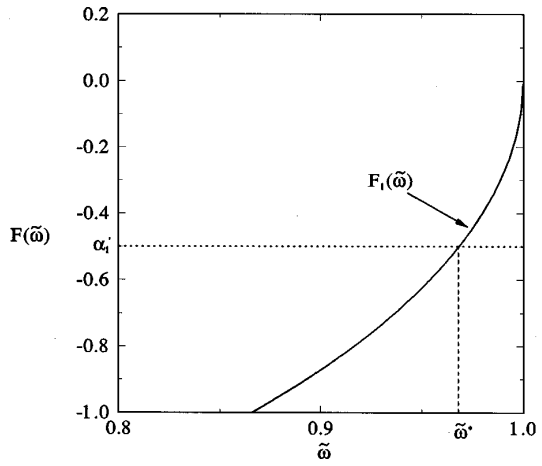

FIG. 1. Graphic solution of Eq. (14), $\alpha_2=0, \alpha_1\neq 0$, $\tilde{M}$ is set to 1, $\tilde{\omega}^*$ is the energy of the bound state.

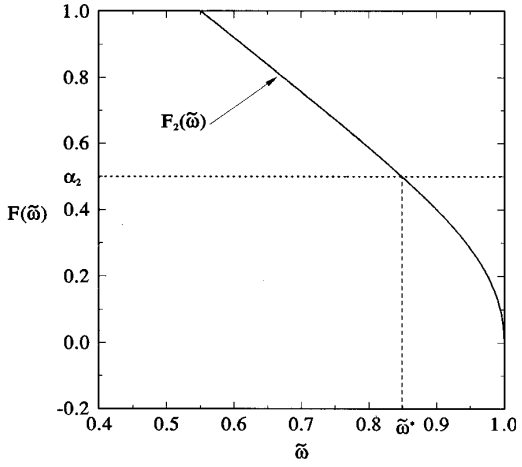

FIG. 2. Graphic solution of Eq. (15), $\alpha_1=0, \alpha_2\neq 0$, $\tilde{M}$ is set to 1, $\tilde{\omega}^*$ is the energy of the bound state.

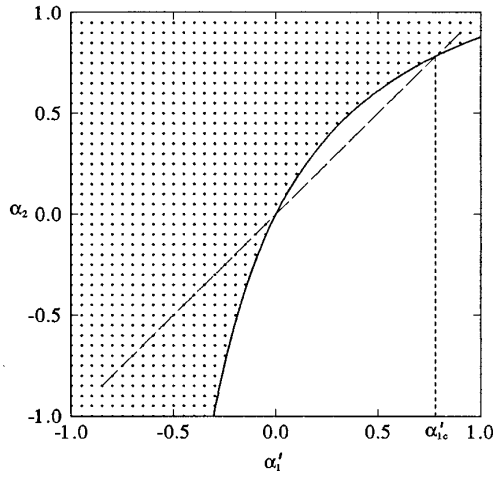

FIG. 3. Graphic solution of Eq. (13), shaded region represents where Eq. (13) exists solution $\omega<M$, $\tilde{M}$ is set to 0.5. The solid curve represents the boundary of the shaded and unshaded regions and the long dashed line represents the assumed relation: $\alpha'_1=\alpha_2$. α'_{1c} shows the threshold (see text).

a bound state, corresponding to an energy level less than M, while in the case of a barrier it cannot appear. Therefore, in order to obtain the bound state the local δ potential must be a well. It can be realized when the coefficient c_1 or c_2 is less than zero, i.e., $\alpha_1<0$ or $\alpha_2>0$ if only a single one of them exists. When these two parameters exist simultaneously there exhibits a competition between them to take on a well or barrier character. Only in some special cases, as shown in shaded region of Fig. 3 can they combine to contribute to a well, which gives rise to a bound state.

There exist relations, as we mentioned before, between the 1D SG model and an $S=1$ Heisenberg spin chain. We may apply the present results to discuss the bound state in a $S=1$ Heisenberg spin chain. Generally speaking, after Jordan-Wigner transformation and bosonization the impurity bond term in spin chain can be transformed into the bosonized form similar to $H_{\rm imp}$ in Eq. (1). But the parameters $\alpha_1(or\ \alpha'_1)$ and α_2 in $H_{\rm imp}$ are now not independent. It is reasonable to think that they are all proportional to $J'-J$, where J' is the impurity bond and J is the exchange coupling. So there exists a proportionality relation between them. In Fig. 3 the assumed line $\alpha'_1=\alpha_2$ is depicted; then we can easily find the possibility of the existence of threshold. In fact, if the slope of the line is within a certain range, the line will always have two intersections with the boundary curve of the shaded and unshaded regions. One is just the origin and the other (it may be beyond the scope of the figure) shows the threshold. For example, in Fig. 3 the threshold for α'_1 is a positive number α'_{1c}. This means when $\alpha'_1<0$ there always exists bound state, while when $\alpha'_1>0$ it does not appear always. Obviously, only when $\alpha'_1>\alpha'_{1c}$ can the region where the bound state appears be reached. This is very similar to the previous results. Reference 5 tells us when $J'-J<0$ the impurity level always appears in the Haldane gap, while when $J'-J>0$ there is a threshold. When the concrete quantitative discussion is carried out, the following two points must be considered: one is that, strictly speaking, there exist minor differences between the impurity bond or its bosonized form and $H_{\rm imp}$ in Eq. (1). The former may embody something else besides the latter, so it needs a generalization about the current Hamiltonian to exactly simulate the impurity bond problem in an $S=1$ Heinsenberg spin chain. Another is that the shaded region in Fig. 3 changes with $\tilde{M}$, which means it is related to the bulk parameters α_0,β_0. A detailed quantitative discussion about the bound state in a spin chain is beyond the present paper, and we leave it for further studies. Nevertheless, we think the Hamiltonian that we have studied in this paper provides a good starting point and gives a simple and clear picture for the study of the impurity problem in a kind of 1D model.

In conclusion, we make use of an analytic self-consistent theory to discuss the bound state in a 1D SG model. We show the possibility of the existence of bound state and find it is decided by two parameters related to impurity terms. Only when these two parameters locate in a definite region can the bound state show up. Furthermore, when these two parameters are not independent, the alternative parameter must exceed some specific value, i.e., threshold value in order to make impurity level exist within the SG global gap.

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