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Commensurate–incommensurate transitions in two dimensions—a low-temperature expansion

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Abstract. The commensurate–incommensurate transition of a two-dimensional classical sine–Gordon system is studied by the equivalent one-dimensional quantum system. The latter is expanded around its classical limit, corresponding to a low-temperature expansion of the two-dimensional system. It is found that both mass and wavefunction renormalisation are required. The critical exponent for incommensurability is $\bar{\beta} = 0$, but if the momentum cut-off is kept finite we obtain $\bar{\beta} = 1$. The classical limit is a singular point and the results are reliable when they are not too close to the transition.

1. Introduction

The commensurate–incommensurate (C–I) transition is of current interest as it generalises the theory of melting in two dimensions. The classical ($T = 0$) theory was solved by Frank and van der Merwe (1949) who showed that the degree of incommensurability vanishes as an inverse logarithm at the transition, i.e. an exponent $\bar{\beta} = 0$. The finite temperature problem can be studied by a one-dimensional quantun sine–Gordon system with quantum coupling $\beta^2 \sim T$ (Takayama 1980). For finite β the exponent is $\bar{\beta} = \frac{1}{2}$, first shown for $\beta^2 = 4\pi$ (Horovitz 1979) and then extended to $0 < \beta^2 < 8\pi$ (Luther *et al* 1979, Pokrovski and Talapov 1979, 1980, Haldane 1980, Schultz 1980). Thus the classical limit $\beta \rightarrow 0$ seems to be a singular point of the theory.

In this paper we study the lowest-order correction in β^2 around the classical limit. This approach is analogous to the spin wave theory of the XY system which can yield information on the transition to the disordered phase (Kosterlitz 1974). Here the corresponding transition is from the incommensurate phase to a fluid phase. The lowest-order correction in β^2 is of further interest as it can be mapped on the adiabatic fermion–phonon system (Horovitz 1981).

2. Renormalisation procedure

Consider the quantum sine–Gordon Hamiltonian

$$H = \int \mathrm{d}x \left(\tfrac{1}{2}\pi^2(x,t) + \tfrac{1}{2}\varphi'^2(x,t) + \frac{m^{*2}}{\beta^2}(1 - \cos\beta\varphi) - \mu \frac{\beta}{2\pi}\varphi'(x,t) \right) \tag{1}$$

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where $\pi = \dot{\varphi}$ and $\dot{\varphi}$, φ' are time and space derivatives respectively. The last term of equation (1) is a chemical potential μ coupled to the soliton density ρ where

$$\rho = \frac{\beta}{2\pi} \int \frac{dx}{L} \langle \varphi'(x, t) \rangle \tag{2}$$

and L is the length of the system.

The C–I transiton occurs when $\mu = E_s$, where E_s is the single soliton energy. Instead of a fixed μ, we consider now a fixed ρ, i.e. a fixed boundary condition on the field. If $\tilde{\psi}_s(x)/\beta$ is a classical solution for the equation of motion, perturbation theory is developed by the substitution $\varphi(x, t) = \beta^{-1}\tilde{\psi}_s(x) + \hat{\varphi}(x, t)$ which yields (Tomboulis 1975, Jackiw 1977):

$$H = \int dx\{(1/\beta^2)[\tfrac{1}{2}\tilde{\psi}_s'^2 + m^{*2}(1 - \cos\tilde{\psi}_s)] + \tfrac{1}{2}\hat{\pi}^2 + \tfrac{1}{2}\hat{\varphi}'^2 + \tfrac{1}{2}m^{*2}\cos\tilde{\psi}_s(x)\,\hat{\varphi}^2\} + O(\beta^2). \tag{3}$$

The translation mode $\tilde{\psi}_s'(x)$ is a degree of freedom of the classical field and is excluded from the field $\hat{\varphi}$, i.e.

$$\int \hat{\pi}\tilde{\psi}_s' \, dx = \int \hat{\varphi}\tilde{\psi}_s' \, dx = 0$$

and

$$i[\hat{\pi}(x, t), \hat{\varphi}(y, t)] = \delta(x - y) - \tilde{\psi}_s'(x)\,\tilde{\psi}_s'(y) \left(\int \psi_s'^2(z)\, dz \right)^{-1}. \tag{4}$$

Since $\tilde{\psi}_s(x)$ is a classical field, its equation of motion is determined by minimising the expectation value $\langle H \rangle$. To order β^2:

$$\tilde{\psi}_s'' + m^{*2}\sin\tilde{\psi}_s - \tfrac{1}{2}\beta^2 m^{*2}\sin\tilde{\psi}_s\langle\hat{\varphi}^2\rangle = 0. \tag{5}$$

For the $\hat{\varphi}$ field equations (3) and (4) yield

$$\ddot{\hat{\varphi}} = \hat{\varphi}'' - m^{*2}\cos\tilde{\psi}_s\hat{\varphi}. \tag{6}$$

The last term of (5) is a mass renormalisation and equation (5) and (6) become non-trivial coupled equations when $\tilde{\psi}_s$ and $\langle\hat{\varphi}^2\rangle$ are space dependent. This difficulty is overcome by a wavefunction renormalisation, i.e. $\tilde{\psi}_s = \psi_s + \psi_1$ where $\psi_1 \sim O(\beta^2)$ and ψ_s is a solution of

$$-\psi_s'' + m_1^2 \sin\psi_s = 0. \tag{7}$$

The renormalised mass m_1 is $m^* + O(\beta^2)$ so that the $\hat{\varphi}$ equation to order β^2 is

$$\ddot{\hat{\varphi}} = \hat{\varphi}'' - m_1^2\cos\psi_s\hat{\varphi}. \tag{8}$$

The function $\psi_1(x)$ can now be determined by expanding equation (5) to order β^2:

$$-\psi_1'' + m_1^2\cos\psi_s \qquad \psi_1 = \tfrac{1}{2}m_1^2\beta^2\sin\psi_s\langle\hat{\varphi}^2\rangle + (m_1^2 - m^{*2})\sin\psi_s. \tag{9}$$

It is shown in the Appendix that $\langle\hat{\varphi}^2\rangle$ can be written in the form $D_s + D_1\psi_s'^2(x)$ for any solution $\psi_s(x)$ of equation (7) where D_s, D_1 are space independent. It is then easy to check that

$$D_s = \left[1 - \frac{\psi_s'}{2\psi_s''}\frac{d}{dx}\right]\langle\hat{\varphi}^2\rangle. \tag{10}$$

It is remarkable that equation (9) can be solved explicitly with the result

$$\psi_1(x) = \tfrac{1}{2}\beta^2 D_1 \psi_s''(x) - (\tfrac{1}{2}m_1^2\beta^2 D_s + m_1^2 - m^{*2})\, x\psi_s'(x)/2m_1^2, \tag{11}$$

The only restriction on ψ_1 is that it should not change the boundary condition, and the crucial observation is that this can be achieved by a suitable choice of m_1. The boundary conditions are $\psi_s(L) - \psi_s(0) = 2\pi\rho L$ and periodic boundary conditions on derivatives of ψ_s, e.g. $\psi_s'(0) = \psi_s'(L)$. Only the second term of equation (11) violates the boundary conditions; therefore we require its coefficient to vanish:

$$m_1^2 = m^{*2} - \tfrac{1}{2}m_1^2\beta^2 D_s + \mathrm{O}(\beta^4). \tag{12}$$

The renormalisation of the vacuum $\psi_s \equiv 0$ involves $D_0 = \langle\hat{\varphi}^2\rangle_0$ which is space independent. The renormalised mass m_0 is then given by:

$$m_0^2 = m^* - \tfrac{1}{2}m_0^2\beta^2 D_0 + \mathrm{O}(\beta^4) \tag{13}$$

in agreement with the normal ordering procedure for renormalising the sine–Gordon system (Coleman 1975). The normal ordering procedure is not sufficient to renormalise space-dependent solutions and $\langle\hat{\varphi}^2\rangle$ has to be replaced by D_s of equation (10). Amit *et al* (1980) have shown that wavefunction renormalisation is also necessary near the point $\mu = 0$, $\beta^2 = 8\pi$. This completes the renormalisation procedure, and we turn now to examine its consequences.

3. Soliton lattice

The solution of equation (7) with a soliton density ρ, also known as a soliton lattice, is given by Frank and van der Merwe (1949):

$$\sin \tfrac{1}{2}(\psi_s - \pi) = \mathrm{sn}(m_1 x/k, k) \tag{14}$$

where sn is the Jacobian elliptic function (Whittaker and Watson 1962) with parameter $k, 0 \leqslant k \leqslant 1$. The solution $\psi_s(x)$ increases by 2π as x is increased by $l = 1/\rho$ where

$$\rho = m_1/[2kK(k)] \tag{15}$$

and $K(k)$ is the complete elliptic integral of the first kind.

Proceeding now to the quantun perturbation, we note that equation (8) describes small oscillations, i.e. phonons, around the classical solution. Equation (8) with ψ_s given by equation (14) corresponds to the Lamé equation and has well known eigenfunctions (Fetter and Stephen 1968, Sutherland 1973). The potential cos $\psi_s(x)$ is periodic, with the first Brillioun zone at the wavevector $q = \pi/l$ and $l = 1/\rho$. The spectrum has a gap just at the first zone and separates the phonons into 'acoustic' and 'optic' branches.

Details of the eigenfunctions and eigenvalues are given in the Appendix. A straightforward calculation now yields:

$$D_s = -\frac{1}{2\pi}\ln\frac{k}{1-k'} + \frac{1}{2\pi}\ln\frac{2}{\varepsilon k} - \frac{1}{2\pi}\frac{1+k'^2}{12}\varepsilon^2 + \mathrm{O}(\varepsilon^4) \tag{16}$$

where $k'^2 = 1 - k$ and $\varepsilon \to 0$ as $\Lambda \to \infty$ (equation A.6).

The vacuum is defined by $\psi_s \equiv 0$ (no solitons) and its phonons have the dispersion

$$\omega_q^0 = (m_0^2 + q^2)^{1/2} \tag{17}$$

where $0 \leqslant |q| < \Lambda$ and $D_0 = \Sigma(2\omega_q^0)^{-1}$. From equations (12) and (13) we derive m_1 which depends on the soliton density through the parameter k:

$$m_1^2 = m_0^2\left\{1 + \frac{\beta^2}{4\pi}\left[\ln\frac{k}{1-k'} + \varepsilon^2\left(\frac{E(k)}{K(k)} - \tfrac{1}{2}k'^2\right) + O(\varepsilon^4)\right]\right\}. \tag{18}$$

In the limit of a single soliton $\rho \to 0$, $k' \to 0$ and $K(k) \to \ln 4/k' \to \infty$ we obtain $m_1 = m_0$. This justifies the renormalisation procedure for a single soliton (Dashen *et al* 1975, Maki and Takayama 1979). In the field theory limit one takes $\varepsilon \to 0$, (or $\Lambda \to \infty$) after cancelling the divergences. In equation (18) we also keep an ε^2 term since it drastically changes the behaviour for $\rho \to 0$: $k' \to 4\exp(-m_1/2\rho)$ while $E/K \to 2\rho/m_1$. This may be relevant to the theory on a lattice with a finite cut-off, and affects the critical behaviour at the C–I transition as we show in the next section.

The energy of the soliton lattice, E_{SL}, is given by the expectation value of equation (3) relative to that of the vacuum. The first term of equation (3) yields

$$\frac{m_1^2}{k^2K}\left[\frac{4}{\beta^2}(E - \tfrac{1}{2}k'^2K) + D_s(E - k'^2K)\right] \tag{19}$$

where the D_S term comes from the mass renormalisation. The second term of equation (3) is the zero point motion which is $\frac{1}{2}\Sigma_q(\omega_q - \omega_q^0)$. When these terms are combined, all divergences as $\varepsilon \to 0$ cancel and the result in terms of m_0 is:

$$E_{SL}/\rho = \frac{8m_0}{\beta^2 k}(E - \tfrac{1}{2}k'^2K)\left(1 - \frac{\beta^2}{8\pi}\right) + \frac{m_0}{\pi k}\left[(E - \tfrac{1}{2}K)\ln\frac{k}{1-k'} + \tfrac{1}{2}k'K + \varepsilon^2\left(\frac{E^2}{2K} - \tfrac{1}{6}E(1+k'^2) + \tfrac{1}{12}Kk'^2\right)\right] + O(\varepsilon^4, \beta^2). \tag{20}$$

A low-density expansion yields:

$$E_{SL} = \rho[E_s + (4m_0/\pi)\exp(-m_0/2\rho) + \varepsilon^2\rho/m_0 + O(\exp(-m_0/\rho))] \tag{21}$$

where

$$E_s = (8m_0/\beta^2)\,[1 - (\beta^2/8\pi)\,(1 - \tfrac{1}{6}\varepsilon^2)] \tag{22}$$

is precisely the renormalised single soliton energy, as previously obtained for $\varepsilon \to 0$ (Dashen *et al* 1975).

The first term of equation (21) is the energy of ρ free (renormalised) solitons as if they are isolated from each other, i.e. infinitely separated in space. The next terms in equation (21) measure the excess energy required to hold solitons with a small but finite density. This excess energy can be viewed as an effective interaction between solitons, as a function of their mean separations $1/\rho$. For $\varepsilon = 0$ the effective interaction is exponential with range $2/m_0$.

In the classical problem the effective interaction is also exponential (proportional to $\exp(-m_0/\rho)$) but the range is smaller by a factor of 2. When $\varepsilon \neq 0$ the effective interaction becomes long-range, i.e. decays as $1/l$. This unusual effect can be traced back to a reduction in the phase space of the optical phonons from $0 \leqslant |q| < \Lambda$ to $\pi/l \leqslant q < \Lambda$. Since D_s is determined mainly by the optical branch it is smaller than D_0 by a term *linear* with $\pi/l \sim \rho$, which should vanish if the phase space is infinite ($\Lambda \to \infty$). From equations (12) and (13) this term increases m_1 relative to m_0, as is indeed shown in equation (18). The energy for $\rho \to 0$ is dominated by $\rho 8m_1/\beta^2$, and when expressed in terms of m_0 it gives the effective interaction as proportional to $\varepsilon^2\rho$.

4. Critical behaviour

The soliton density ρ is the order parameter of the C–I transition. It is determined by minimising $E_{SL} - \mu\rho$ for a fixed μ. Equation (21) shows that the transition occurs at the renormalised soliton energy $\mu = E_s$. Bak and Fukuyama (1980) derived an approximate result for E_s and claimed that for sufficiently large β^2 quantum fluctuations eliminate the C–I transition. Equation (29), although valid only for small β, indicates that E_s vanishes for $\beta^2 = 8\pi$ (if $\varepsilon = 0$). Coleman (1975) shows that the continuum model is indeed unstable for $\beta^2 > 8\pi$, and it becomes a disordered fluid phase in the lattice model (Amit *et al* 1980, Pokrovski and Talapov 1979).

Near the C–I transition $\rho \sim \ln^{-1}(\mu - E_s)$ (when $\varepsilon = 0$) which corresponds to a critical exponent $\bar{\beta} = 0$. This behaviour describes both the classical limit and the lowest-order quantum correction. As discussed in the Introduction, results for finite β give $\bar{\beta} = \frac{1}{2}$ so that the point $\beta = 0$, $\mu = E_s$ is a singular point.

When $\varepsilon \neq 0$ equation (28) yields $\rho \sim \mu - E_s$, i.e. $\bar{\beta} = 1$. It is interesting to note that $\bar{\beta} = 1$ was obtained already for the classical problem by Pokrovski and Talapov (1980) when the area is bounded. In view of the singularity at $\beta = 0$, it seems that $\bar{\beta} = \frac{1}{2}$ at the C–I transition, while not too close to the transition $\bar{\beta} = 1$.

Finally, we consider the density–density correlation function

$$k(x, t) = \langle \exp\{i\beta[\psi(x, t) - \psi(0, 0)]\}/p\rangle,$$

where p is the order of commensurability (Schultz 1980). Using the β expansion and

$$\langle[\varphi(0, t) - \varphi(0, 0)]^2\rangle = \sum_q 2\,|f_q(0)|^2 \sin^2(\tfrac{1}{2}\omega_q t)/\omega_q \xrightarrow[t\to\infty]{} (\pi k')^{-1} \ln t \tag{23}$$

we obtain $K(0, t) \sim t^{-\eta}$ for $t \to \infty$ with

$$\eta = \beta^2/(2\pi k' p^2). \tag{24}$$

Near the C–I transition $k' \to 0$ and $\eta \to \infty$. The condition for the instability of the commensurate phase towards vortex unbinding and forming a fluid phase is given by $\eta > \frac{1}{4}$ (Kosterlitz 1974, Coppersmith *et al* 1981). Thus the fluid phase is formed when μ is close to E_s or temperature ($\sim\beta^2$) is high.

Schultz (1980) has shown that $\eta = 2/p^2$ at the C–I transition and Coppersmith *et al* (1981) concluded that the transition between commensurate and incommensurate phases is always through the fluid phases if $p^2 < 8$. In contrast, the β^2 expansion yields this situation for any p.

Far from the C–I transition $k' \to 1$ and $\eta = \beta^2/(2\pi p^2)$; this coincides with the result of Schultz (1980) in this limit. The transition to the fluid is now at $\beta^2 = \frac{1}{2}\pi p^2$. For $p = 4$ this coincides with the maximal C–I transition temperature at $\mu = 0$, suggesting that the incommensurate fluid line probably extends to zero temperature only for smaller values of p.

In conclusion, the expansion fails at the C–I transition reflecting a singularity at $\beta = 0$; it becomes reliable not too close to the C–I transition. We hope that further work will extend our results.

The result for the soliton lattice energy shows the equivalence of the adiabatic fermion–phonon system to the lowest quantum correction of the sine–Gordon system. Excluding the $1/\beta^2$ term in equation (20) and the first two terms in the square bracket (which come from the acoustic branch) and multiplying by -2 we obtain precisely the result of the spin $\frac{1}{2}$ fermion problem, including the ε^2 terms (Horovitz 1981). The self-consistency equation of the fermion problem is analogous to equation (5); however there is no analogy to the β expansion. Therefore the procedure and details of the two problems are different and only the final result, e.g. equation (20), shows the equivalence.

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Appendix

We summarise here the eigenfunctions and eigenvalues of equation (8) with ψ_s given by equation (14). The elliptic functions and integrals used below can be found in the book by Whittaker and Watson (1962).

The acoustic branch of the eigenvalues corresponds to $0 \leqslant |q| \leqslant \pi/l$ and is given by

$$\omega_q = \frac{m_1 k'}{k} \mathrm{sn}(\chi, k') \tag{A.1}$$

where $k'^2 = 1 - k^2$ and

$$q = (m_1/k)\,[E(\chi, k') - \chi(1 - E(k)/K(k))] \tag{A.2}$$

so that $0 \leqslant \chi \leqslant K(k')$. The normalised eigenfunctions are

$$|f_q(x)|^2 = \frac{1}{L}\frac{\mathrm{dn}^2(m_1 x/k, k) - k'^2 \mathrm{sn}^2(\chi, k')}{\mathrm{dn}^2(\chi, k') - 1 + E(k)/K(k)}. \tag{A.3}$$

The optic branch corresponds to $\pi/l \leqslant |q| < \Lambda$ (in an extended zone notation) with dispersion

$$\omega_q = \frac{m_1\,\mathrm{dn}(\chi, k')}{k\,\mathrm{cn}(\chi, k')} \tag{A.4}$$

where

$$q - \pi/l = \frac{m_1}{k}\left[\chi\left(1 - \frac{E(k)}{K(k)}\right) - E(\chi, k') + \frac{\mathrm{dn}(\chi, k')\,\mathrm{sn}(\chi, k')}{\mathrm{cn}(\chi, k')}\right] \tag{A.5}$$

and $0 < \chi < K(k') - \varepsilon$. The cutoff Λ on q determines ε by:

$$\Lambda = \frac{m_1}{k\varepsilon}\left[1 + \varepsilon^2\left(\frac{E(k)}{K(k)} - \frac{1 + k'^2}{3}\right) - (1 - k'^2 + k'^4)\,\varepsilon^4/45 + \mathrm{O}(\varepsilon^6)\right]. \tag{A.6}$$

The normalised eigenfunctions of the optic branch are

$$|f_q(x)|^2 = \frac{1}{L}\frac{\mathrm{dn}^2(\chi, k') - \mathrm{cn}^2(\chi, k')\,\mathrm{dn}^2(m_1 x/k, k)}{\mathrm{dn}^2(\chi, k') - \mathrm{cn}^2(\chi, k')\,E(k)/K(k)}. \tag{A.7}$$

Note that $\psi_s'(x) \sim \mathrm{dn}(m_1 x/k, k)$ so that from equations (A.3) and (A.7) $\langle\hat{\varphi}^2(x)\rangle = \Sigma_q |f_q(x)|^2/2\omega_q$ can be written in the form $D_s + D_1\psi_s'^2(x)$ as asserted in § 2. Note also that D_1 is infrared divergent since $\omega_q \to 0$ for $q \to 0$. The space-independent part of (A.3) cancels $1/\omega_q$ so that D_s is infrared convergent. The total energy involves $\Sigma\omega_q$ which is infrared convergent; thus the renormalisation should not involve D_1, as is indeed found in equation (12).

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