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SUMMER SCHOOL
on
LOW-DIMENSIONAL QUANTUM SYSTEMS:
Theory and Experiment
(16 - 27 JULY 2001)

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PRE-TUTORIAL SESSIONS
(11 - 13 JULY 2001)

QUANTUM SPIN CHAINS:
Theory and Experiment

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Quantum Spin Chains

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(on leave from U.B.C)

1) Introduction, $S = \frac{1}{2}$ Chains

2) Haldane gap, $S=1$ Chains
Bose Condensation

Quantum Spin Chains Lecture I:

$S=\frac{1}{2}$ Chains

Introduction

$$H = J \sum \vec{S}_i \cdot \vec{S}_{i+1} \quad [J>0], \quad [S^a, S^b] = i\epsilon^{abc} S^c$$

$$\vec{S}^2 = S(S+1), \quad S = \tfrac{1}{2}, 1, \ldots \qquad (\hbar = 1)$$

classical ($S \to \infty$) ground state:

never the exact groundstate for quantum case

$$H = J \sum_i \left[S_i^z S_{i+1}^z + \tfrac{1}{2}\left(S_i^+ S_{i+1}^- + h.c.\right) \right]$$

↑ flips spins in classical gnd state

- Néel state usually a good approx. in $D \geq 2$ but never in $D=1$
- infrared divergences from Goldstone bosons disorder Néel state

Spin-Wave Theory considers small fluctuation away from Néel state: expand in $1/S$:

$$S^z = \pm(S - a^+a), \quad S^\pm = a^+\sqrt{2S - a^+a} \approx a^+\sqrt{2S} + \dots$$

(+ or − for even or odd sites)

- diagonalize quadratic terms with Bogliubov transformation - gives

$$\omega_k \approx v|k| \quad (k \approx 0)$$
$$\approx v|k-\pi| \quad (k \approx \pi) \qquad v = 2JS$$

now calculate reduction of ordered moment (lowest order in $1/S$ - zero pt. motion)

$$\langle S^z \rangle \approx \pm\left[S - \frac{v}{2}\int \frac{dk}{2\pi\omega_k} + \dots\right]$$

- integral diverges at $k = 0, \pi$ in $D=1$ (only)

log divergence suggests an exponentially large length scale where disorder sets in

$$\xi \approx e^{\pi S}$$

Bosonization in 3 steps

- works simply only in $D=1$ for $S=\frac{1}{2}$

1) Spins → fermions (Jordan-Wigner)

$$S_j^z = \frac{1}{2} - \psi_j^+ \psi_j, \quad S_j^- = e^{i\pi \sum_{l<j} \psi_l^+ \psi_l} \psi_j$$

- this reproduces exact commutators

$S_j^z = \pm \frac{1}{2}$ only (Fermi statistics)

$$\{\psi_j, \psi_k^+\} = \delta_{jk}$$

$$H = J \sum_j \left[(\psi_j^+ \psi_{j+1} + h.c) + \psi_j^+ \psi_j \psi_{j+1}^+ \psi_{j+1} \right]$$

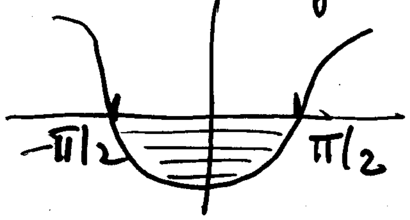
hopping — n.n. repulsion.

2) Continuum limit

- ignore interactions at first

$$\varepsilon_k = -2J \cos k$$

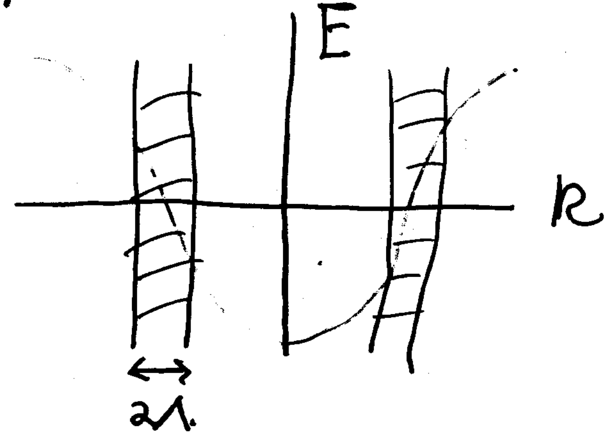
at $\frac{1}{2}$-filling (zero field, $M = \sum S_j^z = 0$)



low energy states only involve

k near $\pm\ \pi/2$

"integrate out" other modes



dispersion relation is approximately linear in low energy theory $\Rightarrow$ Lorentz invariance

$$\psi_j \sim e^{ik_F j}\psi_L(j) + e^{-ik_F j}\psi_R(j) \quad (k_F = \pi/2)$$

$$\mathcal{L} \simeq \psi_R^+ i(\partial_t - v\,\partial_x)\psi_R + \psi_L^+ i(\partial_t + v\,\partial_x)\psi_L$$

- interactions give $\psi_L^+\psi_R\,\psi_R^+\psi_R$ etc.

- now we <u>bosonize</u>

- exact equivalence of Lorentz invariant fermion and boson theories

$\psi_R^+ \psi_R = \frac{1}{\sqrt{4\pi}} (\partial_t + v\partial_x)\varphi$, $\psi_L^+ \psi_L = \frac{1}{\sqrt{4\pi}} (\partial_t - v\partial_x)\varphi$

$\psi_L \propto e^{i\sqrt{4\pi}\,\varphi_L(vt+x)}$, $\psi_R \sim e^{-i\sqrt{4\pi}\,\varphi_R(vt-x)}$

(generally set $v=1$)

$\varphi(t,x) = \varphi_R(t-x) + \varphi_L(t+x)$

$\theta \equiv \varphi_L - \varphi_R$

- the power of bosonization is that it turns interacting fermions into non-interacting bosons, <u>in some cases</u>
- in this case interaction term is essentially proportional to non-interacting term

$\mathcal{L} = \text{const} \cdot \partial_\mu \varphi \partial^\mu \varphi$

- rescale φ to give $\mathcal{L}$ canonical normalization
- we finally obtain asymptotic low energy expressions for orginal spin operators

-the result is a very useful *dictionary* expressing any spin operator in terms of a free massless boson operator whose Green's functions and thermodynamics are easily computed
-only works for low energy long distance behavior however
-the free boson Langrangian in (1+1) dimensions is:

$$L = \left(\tfrac{1}{2}\right)\left[(\partial_t \varphi)^2 - (v_s \partial_x \varphi)^2\right]$$

-v_s is the spin-wave velocity- I often set $v_s = 1$, below
-the dictionary also contains the dual boson, defined by:

$$\partial_t \theta = -\partial_x \varphi, \ \partial_x \theta = \partial_t \varphi$$

-both uniform and staggered components of lattice spin operators are represented by (different) boson operators:

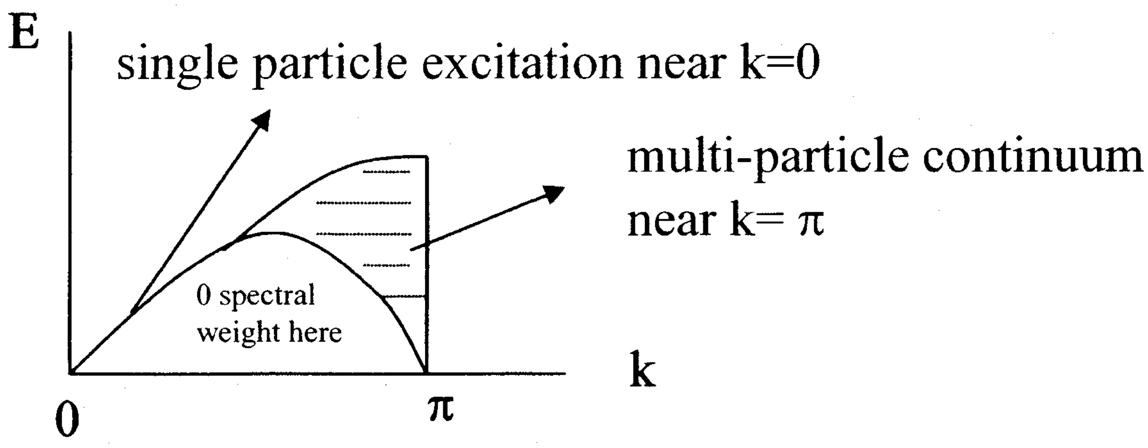
$$S_j^z \approx \frac{1}{2\pi R}\frac{\partial \varphi}{\partial x} + const. \bullet (-1)^j \cos\frac{\varphi}{R}$$

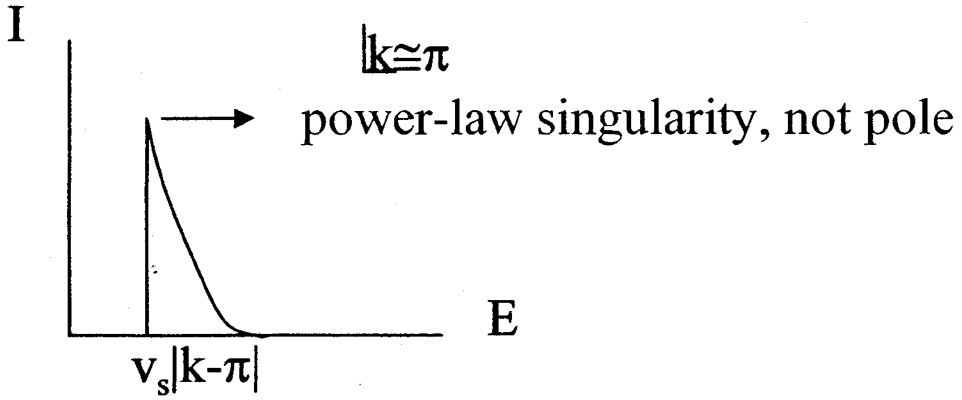
$$S_j^- \approx e^{2\pi i R\theta}\left[const. \bullet \cos\frac{\varphi}{R} + C(-1)^j\right]$$

-here the parameter $R = 1/\sqrt{2\pi}$ but takes other values in general
-note that $(1/2\pi R)\int dx \partial\varphi/\partial x = -(1/2\pi R)\int dx \partial\theta/\partial t$ is the z-component of the conserved total magnetization- this has the right commutator: $\left[S_T^z, S_j^-\right] = -S_j^-$
-it is now straightforward to calculate Green's functions of spin operators near wave-vectors 0 and π
-note that uniform part of S^z is a single boson operator but staggered part is a multi-boson (non-linear) operator
7

-using $<\varphi(x,t)\varphi(0,0>=-(1/4\pi)\ln(x^2-t^2+i\varepsilon)$

we see that staggered S^z correlation function has power law behavior- Fourier transform has multi-boson cut rather than single particle pole





-N.B. by rotational symmetry correlation functions are equal for S^x, S^y, and S^z although this is far from obvious from bosonization formulas

2) Effect of an Applied Magnetic Field

-extra term in Hamiltonian is $-H\sum S_j^z$

-classically spins lie in xy plane and cant in z-direction:

-spectrum still contains a gapless Goldstone mode corresponding to rotations around z-axis

-within bosonization approach:

$$H\sum S_j^z \rightarrow \frac{H}{\sqrt{2\pi}}\int dx \frac{d\varphi}{dx}$$

-we eliminate this term in the Lagrangian by a simple change of variables:

$$\varphi(x) \rightarrow \varphi(x) + \frac{H}{\sqrt{2\pi}}x$$

-so the magnetization is $m(H) = H/\sqrt{2\pi}$

-we still have a massless free boson Lagrangian but:

$$(-1)^j \cos(\varphi/R) \rightarrow \cos[(\pi + H)j + \varphi/R]$$

-i.e. critical wave-vector shifts by ±H for staggered part of S^z, but not staggered part of S^-

- a more careful analysis shows that R varies smoothly as a function of H (as does v_s)

-R(H) v_s(H) are calculable using Bethe ansatz for S=1/2 Heisenberg model

3) What's Special about Cu Benzoate? Staggered H-Field

-in general Zeeman term in Hamiltonian is:

$$H_Z = -\mu_B \sum_{j,a,b} H^a g_j^{ab} S_j^b$$

-in some low symmetry crystals like Cu Benzoate, gyromagnetic tensor, g, has a staggered term:

$$g_j = g_u + (-1)^j g_s$$

-this results from 2 inequivalent Cu ions per unit cell along chain direction (c-axis)
-leads to an effective staggered field, h, approximately perpendicular to uniform applied field, H
-h/H is strongly dependent on direction of applied field
-there is another peculiar, low symmetry exchange interaction that occurs in these crystals (Dzyaloshinski-Moriya)
-this can also be mapped into a staggered field
-other anisotropy is small so we can always define z as uniform field direction and x as staggered field direction

$$Hamiltonian = \sum_j [J\vec{S}_j \bullet \vec{S}_{j+1} + HS_j^z + h(-1)^j S_j^x]$$

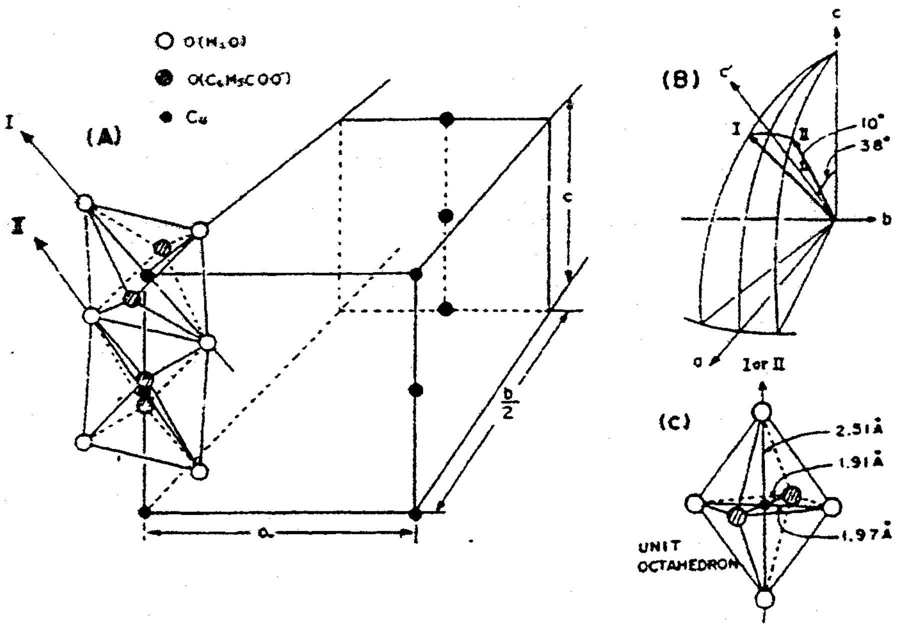


Figure 2.2: Crystal structure of $Cu(C_6H_5COO)_2 \cdot 3H_2O$, copper benzoate. (A) Schematic view of one-half the unit cell. Room temperature lattice constants are a = 6.98 Å, b = 34.12 Å, c = 6.30 Å, and $\beta = 89.5°$. (B) Orientation of the local symmetry axes I and II in (A) arising from the distorted octahedra surrounding each Cu ion. The a'-axis is defined as $\perp$ to the b and c' axes. (C) Unit octahedron, showing the distances between Cu and its ligand atoms. Figure reprinted from Reference [41].

-Goldstone mode now has finite gap semi-classically-
there are only 2 classical groundstates, differing by a π-rotation around z-axis (or translation by 1 site) ground state is unique
-semi-classical excitations are small fluctuations and solitons (π-rotations of staggered magnetization in xy plane)
-bosonization description: uniform field just gives momentum shift but staggered field produces sine-Gordon interaction
-writing L in terms of the dual θ-field:

$$L = \frac{1}{2}\left[(\partial_t \theta)^2 - (\partial_x \theta)^2\right] + hC \cos 2\pi R\theta$$

-as before, the effect of the uniform field, H, is essentially just to shift R, v_s and the critical wave-vector

4) Sine-Gordon Model Quantum Field Theory in (1+1) Dimensions

-non-trivial exact excitation spectrum is known since the semi-classical solution by DHN
-consists of several interacting (stable) massive particles: solitons and "breathers"- i.e. soliton-antisoliton boundstates, depending on value of R [$\beta^2=(2\pi R)^2 \cong 2\pi$]
-in general breathers can be very strongly bound with M_i considerably smaller than $2M_S$
-at small β, the lowest breather may be thought of as the perturbative fundamental boson excitation and the higher breathers as boundstates of it
-at $\beta^2=2\pi$ there is an exact SU(2) symmetry and the lowest breather is degenerate with soliton and anti-soliton, forming a spin triplet and there is a second breather heavier by a factor of $\sqrt{2}$
-as R decreases, both breather masses decrease and a third breather drops below soliton-antisoliton continuum at $2M_S$
-breather states are created from the vacuum by the operators sin ($2\pi R\theta$), cos ($2\pi R\ \theta$), since they are "θ -particles"
-solitons carry charge ± 1 with respect to U(1) symmetry: $\varphi \rightarrow \varphi$+const.
-they are created by exp($\pm i\ \varphi/R$) operators

-the mass scale is determined by renormalization group scaling arguments:

$M_S \propto h^\nu$, with $\nu = 1/(2-\pi R^2) \approx 2/3$

-the model is exactly integrable: infinite number of conserved currents

-exact specific heat C(T) is known: it crosses over from massless boson behavior at $T >> M_S$: $C = (\pi/6v)T$, to massive boson behavior at $T << M_S$: $C = (M^3/2\pi T^5)^{1/2} e^{-M/T}$ (where M is mass of lightest breather)

-from exact F(h,T) we can also determined staggered susceptibility, $\partial^2 F / \partial h^2$

-exact form factors are known

-for $R \leq \sqrt{2\pi}$, the first breather form factor is much bigger than higher breathers (perturbative behavior)

5) Back to Cu Benzoate

a) Specific Heat (O&A, Essler)

-specific heat changes from linear to exponential in finite field

-gap scales as $H^{2/3}$,

-as expected, there is strong dependence on field direction since h/H depends on field direction

-detailed form of C(T) agrees quite well with S-G model

b) Neutron Scattering

-in zero field there are no single particle peaks- just power law singularities

-at finite H we see expected momentum shift $\pi \rightarrow \pi \pm H$

-we also see resolution limited single particle peaks

-different mass gaps at wave-vector π, corresponding to $S^{\pm}$ Green's function (breather) and $\pi \pm H$ corresponding to S^z Green's function (soliton)

M_B/M_S=.79 for πR^2=.41, predicted by S-G model

-this value of R is expected for Heisenberg model for $g\mu_B H/J$=.52 (H = 7 Tesla, J=1.57 meV) from Bethe ansatz

-soliton is also visible at wave-vector π, but at energy

$E = \sqrt{M_S^2 + H^2}$ due to momentum shift by H

F. Essler

FIG. 4. Specific heat as a function of temperature for fields of H=3.5T and H=7T applied along the c'' axis .

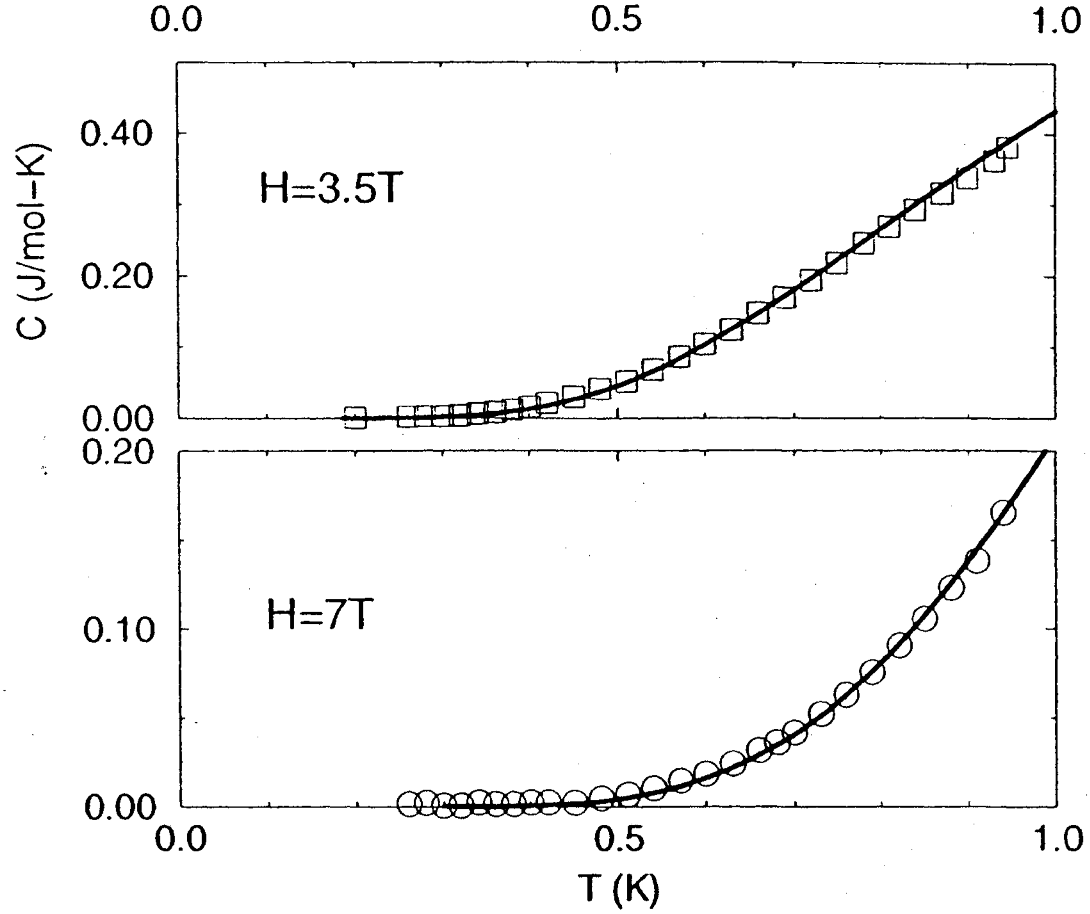


FIG. 5. Specific heat as a function of temperature for fields of H=3.5T and H=7T applied along the c'' axis. The spin velocity is taken to be eight percent smaller than in the MM

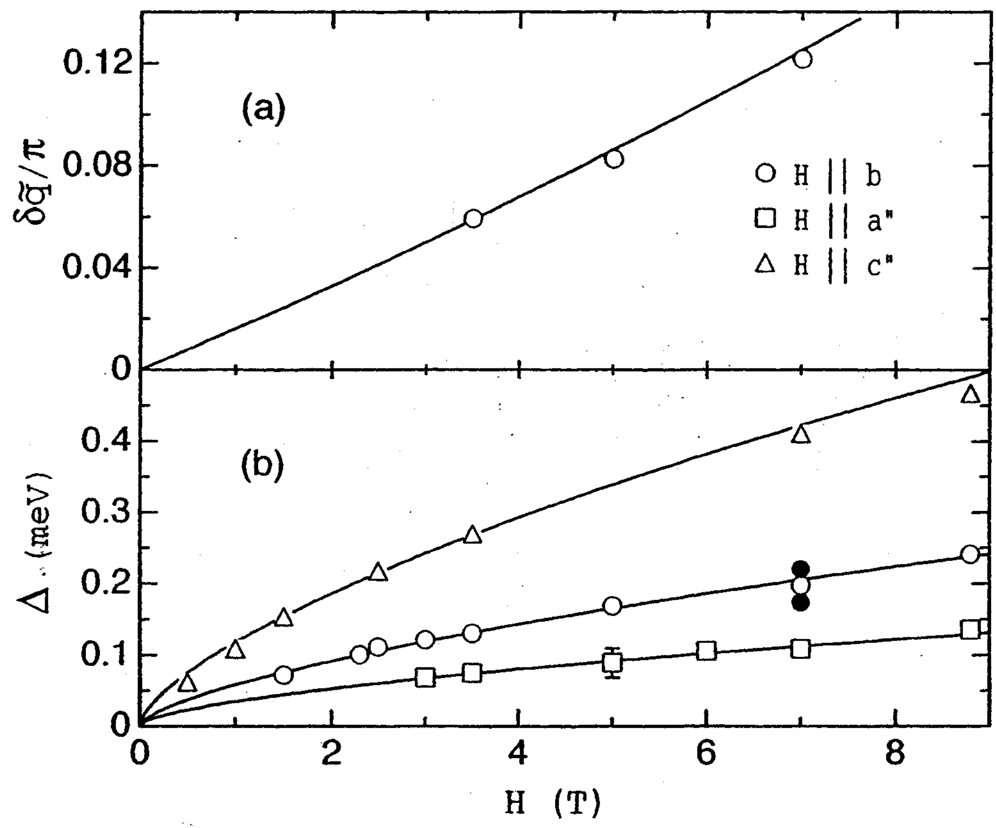


Figure 6.14: (a) Field dependence of the displacement $\delta\tilde{q}$ of the incommensurate side peaks from $\tilde{q} = \pi$ in copper benzoate, as derived from fits to the data shown in Fig. 2. The solid line is the theoretical curve from Ref. [21]. (b) Field dependence of the energy gap derived from fits to specific heat data such as those shown in Fig. 4. Data for fields along the three principal magnetic directions are shown. Filled symbols are the gaps measured at $\tilde{q} = \pi$ and $\tilde{q} = 1.12\pi$ by neutron scattering. The solid lines are from fits to power-laws described in the text.

Dender et al.

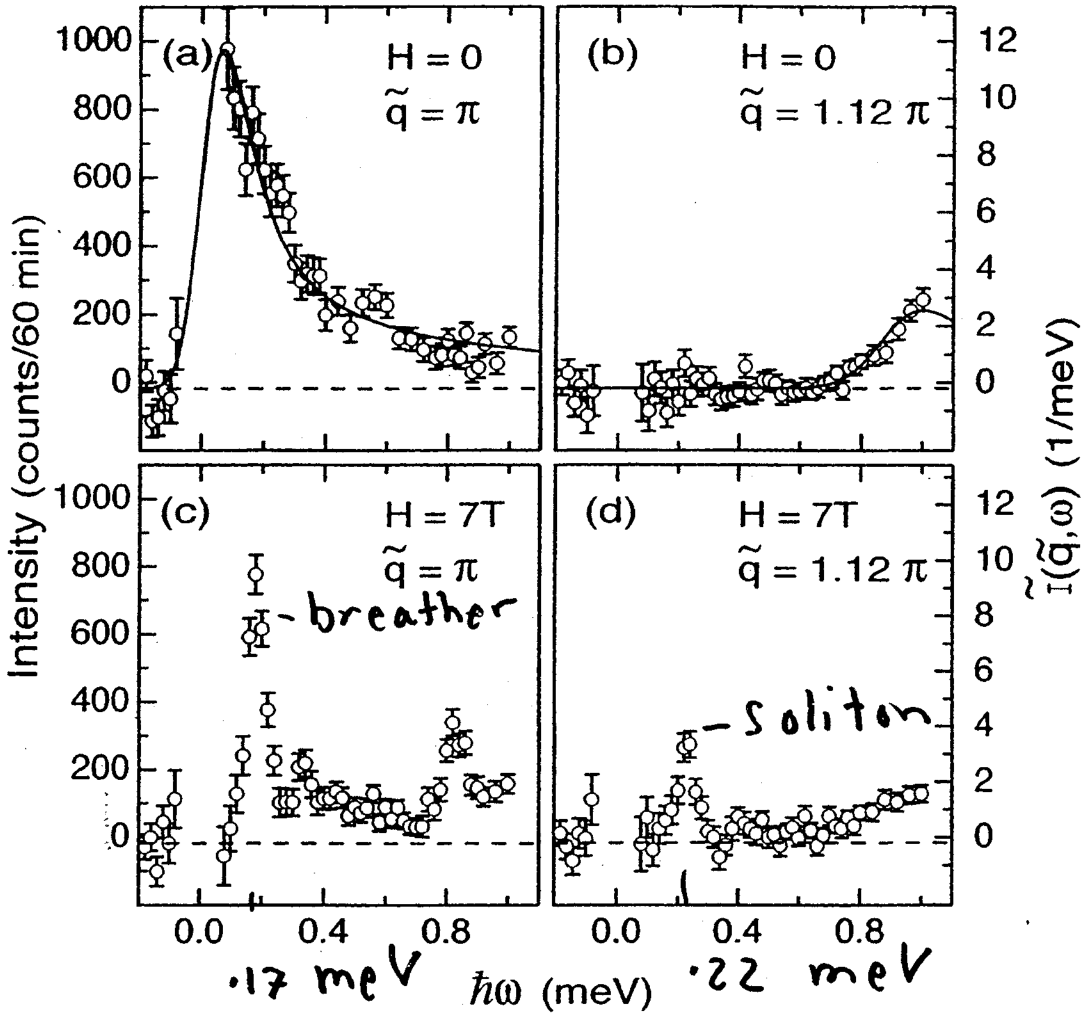


Figure 6.8: Energy dependence of the magnetic scattering intensity at $T = 0.3$ K for $\mathbf{Q} = (0.3, 0, 1)$ and $\mathbf{Q} = (0.3, 0, 1.12)$ at $T = 0.3$ K. The latter wave vector corresponds to the position of the incommensurate maxima in the $H = 7$ T constant-$\hbar\omega = 0.21$ meV scan. The solid lines through the $H = 0$ T data are the theoretical dynamic correlation function [23] convolved with the experimental resolution. The dashed lines are the average of the data in (b) for 0.08 meV $< \hbar\omega <$ 0.6 meV, which is a good measure of the over-subtraction caused by isotropic magnetic scattering contained in the $T = 25$ K data used as a background.

described in the last section and in Chapter 5.

The spectrum changes dramatically for $H = 7$ T, as shown in Fig. 6.8(c) and Fig. 6.8(d). At $\tilde{q} = \pi$, there is no magnetic scattering for $\hbar\omega < 0.1$ meV, indicating that a gap has developed in the spectrum. Above this gap, a sharp, resolution-limited mode peaked at $\hbar\omega = 0.17$ meV now marks the onset of the continuum. A second, resolution-limited mode also appears at $\tilde{q} = \pi$ at an energy close to the Zeeman energy $g\mu_B H = 0.81$ meV. Figure 6.8(d) reveals that at $H = 7$ T, the

c) Electron Spin Resonance

-adsorption of microwave radiation via Zeeman coupling, proportional to zero wave-vector Green's function

-corresponds to $\partial_x\theta$ Green's function at wave-vector H in bosonized theory

-at T>>M this is essentially just free massless boson Green's function- cosine interaction negligible

-gives a δ-function peak at E=H

-as T is lowered, the S-G interaction can be treated, at first, in perturbation theory

-in second order it produces a finite width and shift of this peak: width $=.7Jh^2/T^2$

-width increases as T is lowered and S-G interaction becomes more important

-at T<<M, perturbation theory in S-G interaction is infrared divergent and non-perturbative behavior of S-G model must be taken into account:

-$\partial_x\theta$ creates breather (plus negligible multi-particle continuum)

-breather peak occurs at $E=\sqrt{M_B^2+H^2}$

-peak width goes to zero as exp (-M/T) at low T since only collisions with thermally activated particles produce broadening

Formalism for ESR Calculations

in standard (Faraday) experiments constant field is in $\hat{z}$-direction, alternating field is in xy plane

$$I(\omega) \propto \mathrm{Im} \langle S^\alpha S^\alpha \rangle_{Ret} (\omega, k=0)$$
$$(\alpha = x \text{ or } y)$$

after eliminating magnetic field in bosonized theory by momentum shift we can make a rotation and calculate instead: $\langle S^z S^z \rangle_{Ret} (\omega, k = H)$

(staggered field, or other perturbation, must also be rotated)

$$I \propto \mathrm{Im} \langle \partial_x \varphi \, \partial_x \varphi \rangle_{Ret} (\omega, k = H)$$

$$\propto \mathrm{Im} \frac{H^2}{\omega^2 - H^2 - \Pi(\omega, k=H) - i\epsilon}$$

in favourable cases we can calculate self-energy, Π, perturbatively in staggered field or other symmetry-breaking perturbations

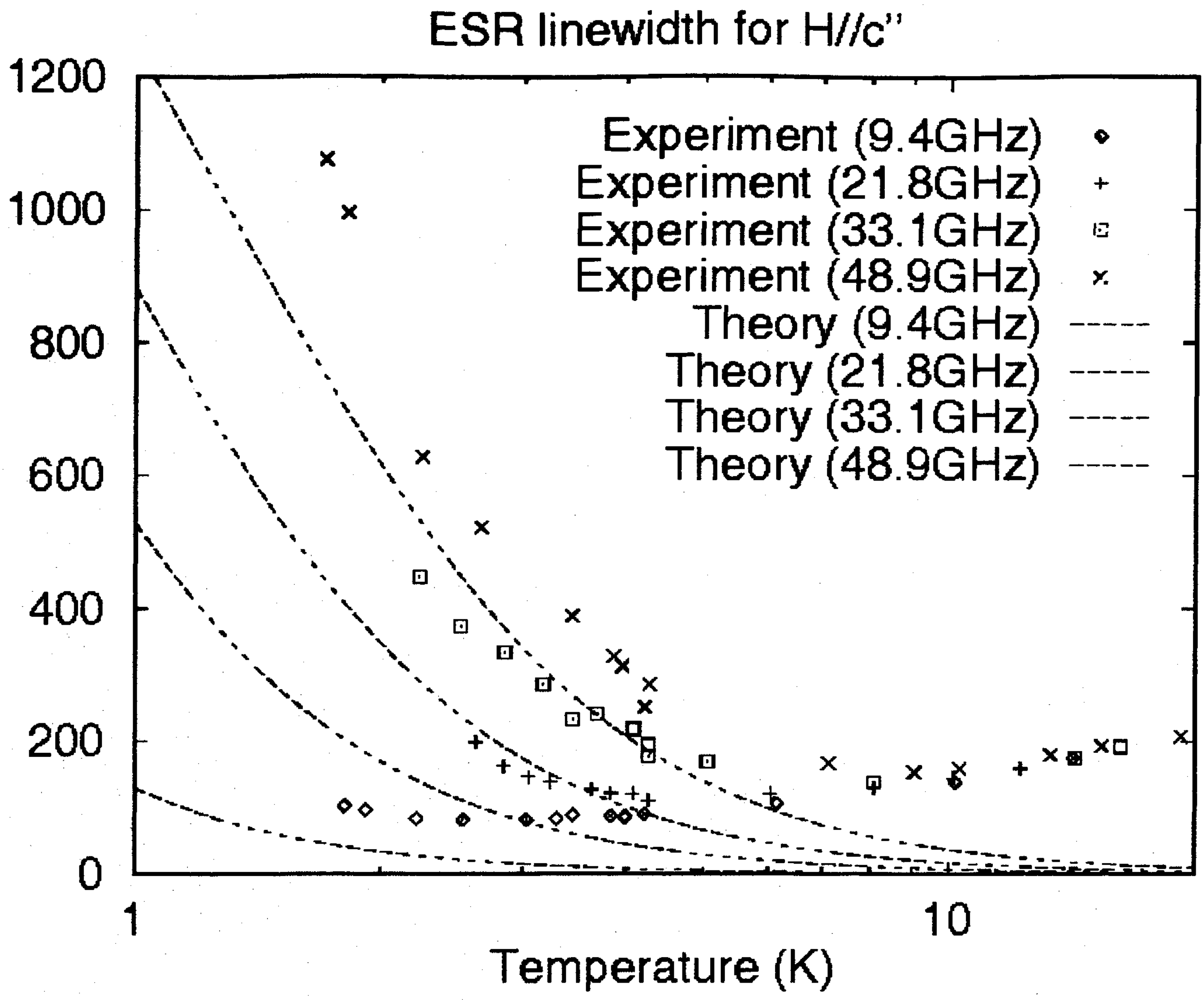
$$\text{width} = -\frac{1}{2H}\,\mathrm{Im}\,\Pi(\omega = H, k = H)$$

for small, smoothly varying, Π

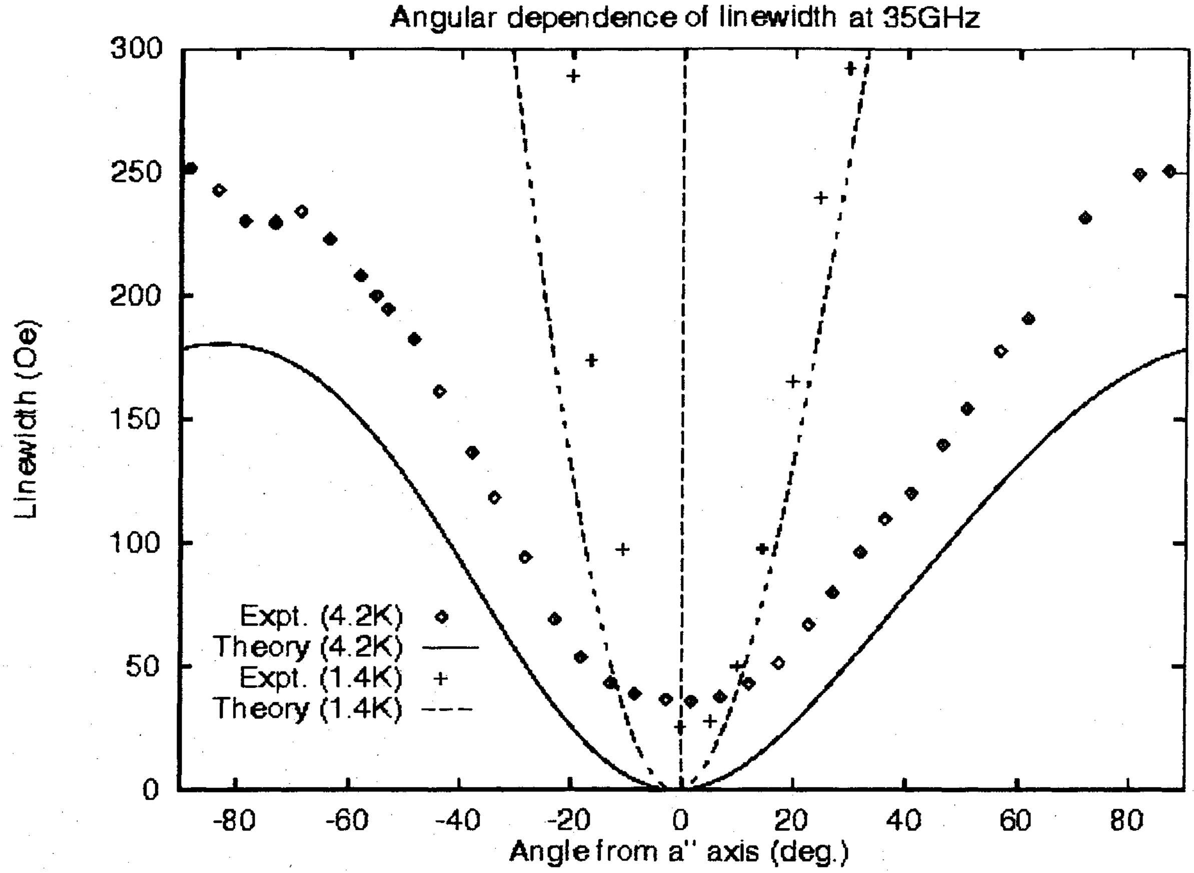
- in this case line shape is Lorentzian

$$I \propto \frac{1}{(\omega - H)^2 + (\text{width})^2}$$

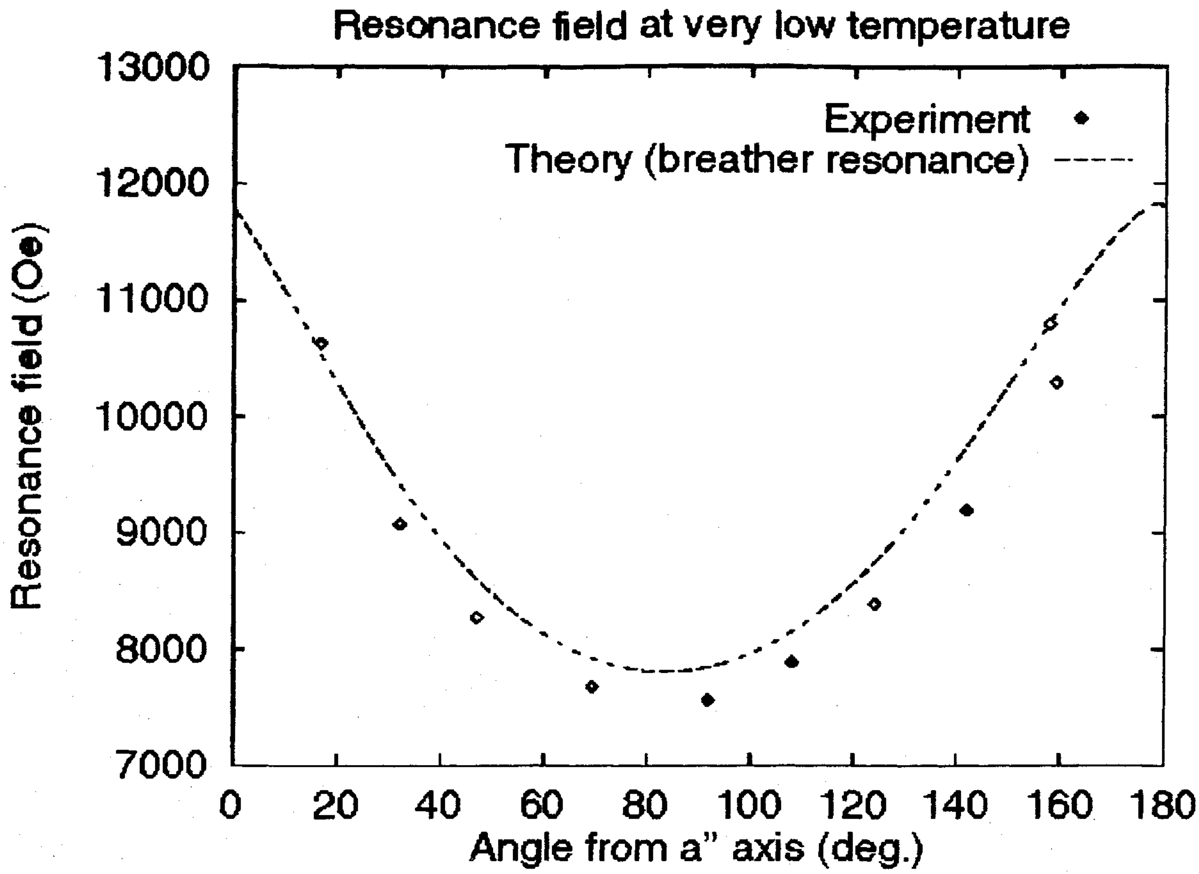
(there is also a shift of peak $\propto \mathrm{Re}\,\Pi$)



-temperature and frequency dependence of ESR line width for H// c″ compared to our theory based on staggered field broadening: $\eta \propto h^2/T^2$
-although the agreement is not too bad at low T there is clearly another contribution to the width which *increases* with T at higher T



The field-direction dependence and magnitude of the line-width in Cu benzoate are roughly reproduced by our theory based on the staggered field anisotropy. According to our theory, the staggered field vanishes when the applied field is along the a″ axis, so the width vanishes in that case There must be some other kind of anisotropy producing a small width for that field direction.



The angular dependence of the resonance field at very low T agrees with the angular dependence of the energy of the breather,

$$\omega = \sqrt{H^2 + \Delta(h)^2}$$

which arises from the *angular dependence of the staggered field*, h.

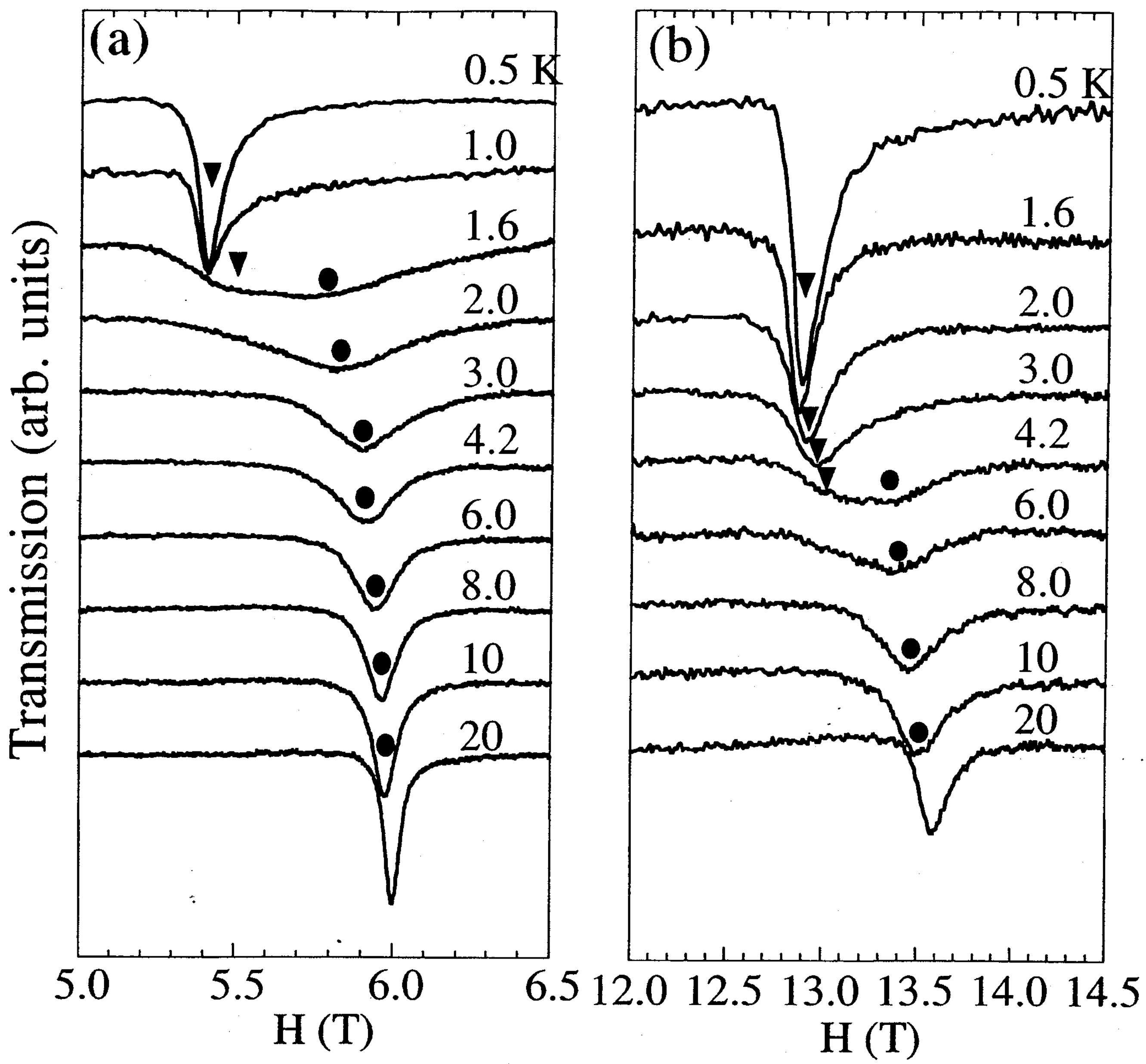


Fig. 1 Asano et al.

References for 1st lecture

$S=\frac{1}{2}$ chains - bosonization etc.

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SU(2) symmetry of $\beta^2 = 2\pi$ Sine-Gordon Model

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Quantum Spin Chains

Lecture 2: Haldane gap, S=1 chains

1. Non-linear σ-model
2. S(q, ω): 1, 2, 3 magnon terms
3. Effect of a uniform field: Bose condensation, magnon-magnon interactions
   - comparison with exact results on σ-model

- bosonization approach can be extended to larger S but it gets complicated and less predictive
- an alternative approach, based on large-S limit, turns out to be very useful even for $S=1$ (and mainly for integer-S)
- it can also be easily extended to 2 or 3D case, unlike bosonization
- based on simplification of commutation relations at large-S
- again it is an approach based on low energy, long-wavelength effective Hamiltonian

well with the numerical results for k close to 0. For $k/\pi \geq 0.1$ the free-boson estimate for the two magnon part of $S(k)$ is larger than the numerical results for the full structure factor. Since the free-boson theory does not take interaction effects into account this is perhaps not too surprising.

In Figs. 13 and 14 are also shown the inelastic neutron scattering (INS) results of Ref. 18, which are directly comparable to our results. The open triangles are points where to within experimental accuracy $S^{\parallel}$ and $S^{\perp}$ were identical. The full squares and circles are data points where $S^{\parallel}$ and $S^{\perp}$, respectively, could be resolved experimentally. Good agreement is obtained with the experiment apart from an overall scale factor of about 1.25, which was to be expected, since the experimental total intensity exceeded the exact sum rule: $(1/L)\sum_{\alpha\tilde{k}} S^{\alpha\alpha}(\tilde{k}) = s(s+1)$ by 30% (± 30%). A very nice agreement between the numerical results and experimental data is evident.

Figure 15 summarizes our results for $S^{\parallel}$ and $S^{\perp}$. In this figure the two structure factors are plotted together with the different theoretical estimates. For the range $(0.1-0.85)k/\pi$ $S^{\parallel}$ is the larger of the two, and only when $k/\pi \geq 0.85$ or $k/\pi < 0.1$ does $S^{\perp}$ become dominant. The crossing of the two structure factors near $k/\pi \sim 0.85$ is correctly described by the SRL if different velocities for the two modes are allowed for. The crossing near $k/\pi \sim 0.1$ seems also to be predicted by the free-boson theory estimate for the two-magnon part of the structure factor. This seems also to be supported by exact diagonalization studies for $L = 16$.[24]

In the case of the *isotropic* chain, with $D = 0.0$, it is possible to obtain an exact expression for the two-magnon part of $S(k\omega)$ within the framework of the NLσ model,[46] thereby taking into account interaction effects. In Ref. 46 it is shown that with $S = S^x = S^y = S^z$, the two-magnon contribution to S is given by

$$|G(\theta)|^2 \frac{vk^2}{2\pi} \frac{\sqrt{\mathbf{K}\cdot\mathbf{K} - 4\Delta^2}}{(\mathbf{K}\cdot\mathbf{K})^{3/2}}, \quad \mathbf{K}\cdot\mathbf{K} > 4\Delta^2. \qquad (6.10)$$

Here $\mathbf{K}\cdot\mathbf{K} = 4\Delta^2\cosh^2(\theta/2)$ and $|G(\theta)|^2$ is given by the expression

$$|G(\theta)|^2 = \frac{\pi^4}{64} \frac{1 + (\theta/\pi)^2}{1 + (\theta/2\pi)^2} \left(\frac{\tanh(\theta/2)}{\theta/2}\right)^2. \qquad (6.11)$$

This calculation contains no free parameters. The expression for the two-magnon contribution to $S(k,\omega)$ can now easily be integrated numerically over ω to obtain $S(k)$. Our numerical results are shown in Fig. 16 along with the SRL form using the previously obtained values for v, g, and ξ. The SRL form is shown as the short-dashed line. Also shown, as the solid line, is the NLσ model results for the two-magnon part of $S(k)$. As seen in Fig. 16 there is excellent agreement between the theoretical and numerical results. The long-dashed line is the prediction from the free-boson theory for the two-magnon contribution to the structure factor. The inclusion of interaction effects changes the shape of $S(k)$, and we see that the free-boson estimate, although qualitatively correct near $k = 0$, somewhat overestimates $S(k)$ for larger k. Presumably the NLσ model also predicts a four-magnon (and higher) contribution to $S(k,\omega)$. This is not known exactly and not included in Eq. (6.10). Hence, the full $S(k)$ in the NLσ model should be somewhat larger than Eq. (6.10). The very precise agreement with the numerical results may indicate that this multimagnon contribution is very small. Alternatively, it may indicate that the NLσ model somewhat overestimates the two-magnon part. Our numerical results for $S(k)$ are also in good agreement with previous results using Monte Carlo techniques[30,31] for chains of length 64.

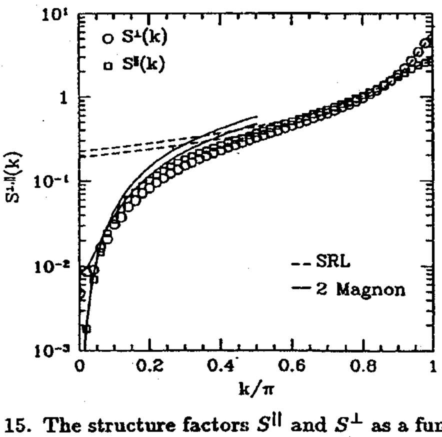


FIG. 15. The structure factors $S^{\parallel}$ and $S^{\perp}$ as a function of k/π for a 100-site *anisotropic* chain. The numerical results are shown as open squares and circles, respectively. The dashed lines are the SRL form obtained by fitting close to $k = \pi$. The solid lines are the predictions from the free-boson theory for the contribution to the structure factor stemming from two-magnon excitations.

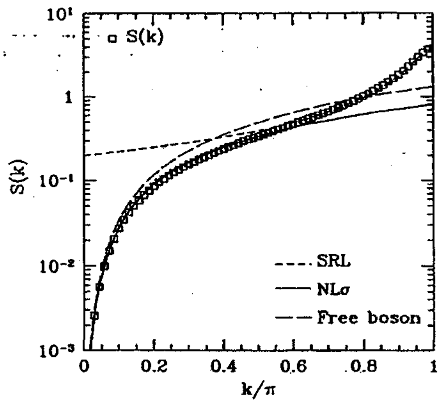


FIG. 16. The structure factor S as a function of k/π for a 100-site *isotropic* chain. The numerical results are shown as open squares. The short-dashed line is the SRL form obtained by fitting close to $k = \pi$. The solid line is the exact prediction from the NLσ model for the contribution to the structure factor from two-magnon excitations. The long-dashed line is the free-boson prediction for the two-magnon contribution to the structure factor.

- express $\vec{S}_j$ in terms of uniform and staggered parts:

$$\vec{S}_j \approx \vec{l} + (-1)^j s\, \vec{\varphi}$$

where $\vec{l}$ and $\vec{\varphi}$ vary slowly, $\vec{\varphi}^{\,2} = 1$, $\vec{l} \cdot \vec{\varphi} = 0$

at large-S the $\vec{S}_j$ commutation relations are approximately reproduced by:

$$[l^a(x), l^b(y)] = i\epsilon^{abc} l^c(x)\, \delta(x-y)$$

$$[l^a(x), \varphi^b(y)] = i\epsilon^{abc} \varphi^c(x)\, \delta(x-y)$$

$$[\varphi^a(x), \varphi^b(y)] = 0$$

- these are commutation relations and constraints of a well-studied Lorentz invariant quantum field theory O(3) non-linear σ-model

- substituting these expressions into original lattice Hamiltonian gives the approximate low energy Hamiltonian:

$$H \approx v \int dx \left[\frac{g}{2} \vec{\ell}^{\,2} + \frac{1}{2g} \left(\frac{d\vec{\varphi}}{dx} \right)^2 \right]$$

$v = 2JS, \quad g = \frac{2}{S}$

- this is H of NLσM

- Corresponding Lagrangian:

$$\mathcal{L} = \frac{1}{2g} \left[\left(\frac{\partial \vec{\varphi}}{\partial t} \right)^2 - \left(\frac{\partial \vec{\varphi}}{\partial x} \right)^2 \right], \quad \vec{\varphi}^{\,2} = 1$$

with v set equal to 1 again

$$\vec{\ell} = \frac{1}{g} \vec{\varphi} \times \frac{\partial \vec{\varphi}}{\partial t}$$

- actually, this isn't quite the whole story, even at large-S

- there is an additional topological term

4.

- this is a term in H which can be removed by a canonical transformation

$\propto \; S\, \vec{l} \cdot d\vec{\varphi}/dx$

or a term in $\mathcal{L}$ which is a total derivative:

$$\mathcal{L} \to \mathcal{L} + \frac{\theta}{4\pi}\, \epsilon^{\mu\nu}\, \vec{\varphi} \cdot (\partial_\mu \vec{\varphi} \times \partial_\nu \vec{\varphi}), \quad \theta = 2\pi S$$

- this term can be derive at the Hamiltonian level by method outlined above or at the Lagrangian / path integral level by writing path integral for a single spin, involving a "Berry's phase" term and then taking continuum limit

- even though top. term is a total derivative, it can't be ignored this can be seen from imaginary time Feynman path integral with 2D space-time compactified on a sphere (circle at $\vec{x} \to \infty$ identified as a point)

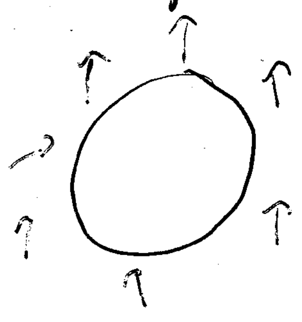
$$Z = \int [d\vec{\varphi}]\, e^{-S_0 + i\theta Q}$$

$$S_0 = \frac{1}{2g}\int d^2x\, (\partial_\mu \vec{\varphi})^2, \quad Q = \frac{1}{4\pi}\epsilon^{\mu\nu}\int d^2x\, \vec{\varphi}\cdot(\partial_\mu\vec{\varphi}\times\partial_\nu\vec{\varphi})$$

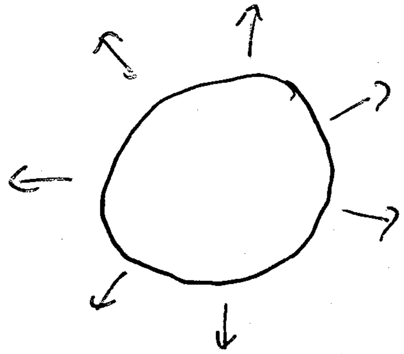
Q is integer-valued topological charge

$\vec{\varphi}$ represents a pt on a sphere, as does $\vec{x}$

Q measures "winding number" of sphere onto sphere



$Q = 0$



$Q = 1$

Q is an integer for any smooth $\vec{\varphi}(\vec{x})$

$\therefore\ \theta$ is an angle: $\theta \leftrightarrow \theta + 2\pi n$

since $\theta = 2\pi S$, topological term has no effect for S = integer but must be retained for S = $\frac{1}{2}$- integer

$\theta = 0$ model is very well understood from its exact integrability, together with large-N limit of $O(N)$ σ-model and renormalization group arguments

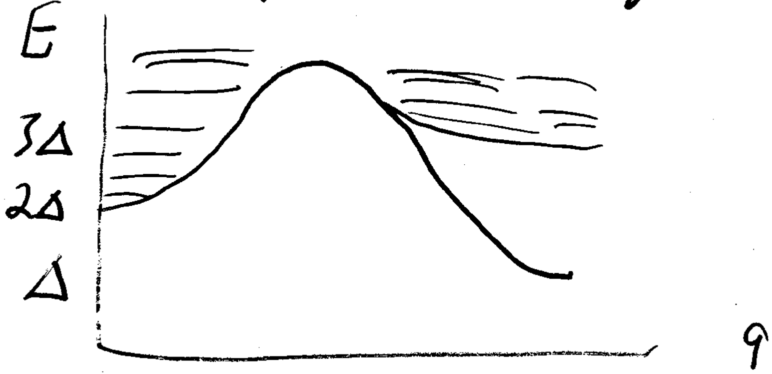
- this model has a mass gap
- spectrum is a <u>triplet</u> of <u>massive</u> bosons $\vec{\varphi}\,|0\rangle$
- they have <u>repulsive</u> <u>interactions</u> and do not form boundstates
- exact form factors and free energy are known

since $\vec{S}_j \simeq \frac{1}{g} \vec{\varphi} \times \frac{\partial \vec{\varphi}}{\partial t} + (-1)^j s \vec{\varphi}$,

$\vec{S}(q)$ creates single magnon at $q \approx \pi$

$$E \approx \sqrt{\Delta^2 + v^2 (q-\pi)^2}$$

but 2 magnons at $q = 0$



- qualitative features of these predictions agree with experiments and numerical simulations for $S=1$, even

$\Delta \approx .4 J$, $\xi = \frac{v}{\Delta} \approx 6$

experiments on N.E.N.P., an $S=1$, Ni^{2+} compound have observed single magnon xcitation near $q=\pi$ (neutron scattering)

triplet is split into doublet and singlet due to crystal field anisotropy:

$$\delta H = D \sum_j (S_j^z)^2 \sim D \int dx \, (\varphi^z)^2$$

destroys integrability of NLσM)

- detailed form of $S(q,\omega)$ at $q \approx 0$ predicted by NLσM because 2-boson form factor is known exactly

$$\langle 0 | \ell^a(q) | q_1, b; q - q_1, c \rangle$$

- since groundstate is a spin singlet, $\langle 0 | \ell^a(q=0) = 0$

$$S(q,\omega) \sim q^2 \quad \text{at } q \to 0$$

- weak signal difficult to see in neut. scatt.

NLσM prediction agrees very well with D.M.R.G. results for equal-time correlation fnc.: $\int d\omega\, S(q,\omega)$ but not so well for $S(q,\omega)$ itself

(T. Kuehner et al. ~~unpublished~~ ?)

- 3 magnon contribution near $q=\pi$ can also be predicted by NLσM
- it is very small (~2% of single magnon part)
- a much bigger $S(\pi,\omega)$ extending all the way down to $\omega=\Delta$ (rather than 3Δ as expected) was observed recently in $CsNiCl_3$
- this is presumably due to significant inter-chain coupling ($J'/J \sim .03$) which produces Néel order at low T

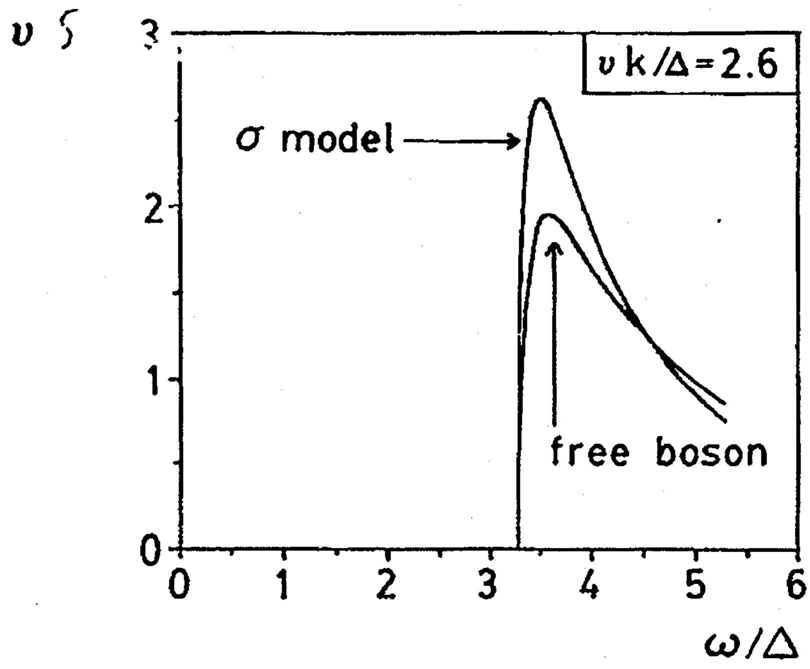


FIG. 1. $S(\omega,k)$ for $k=2.6\Delta/v$ from the free-boson an nonlinear σ models.

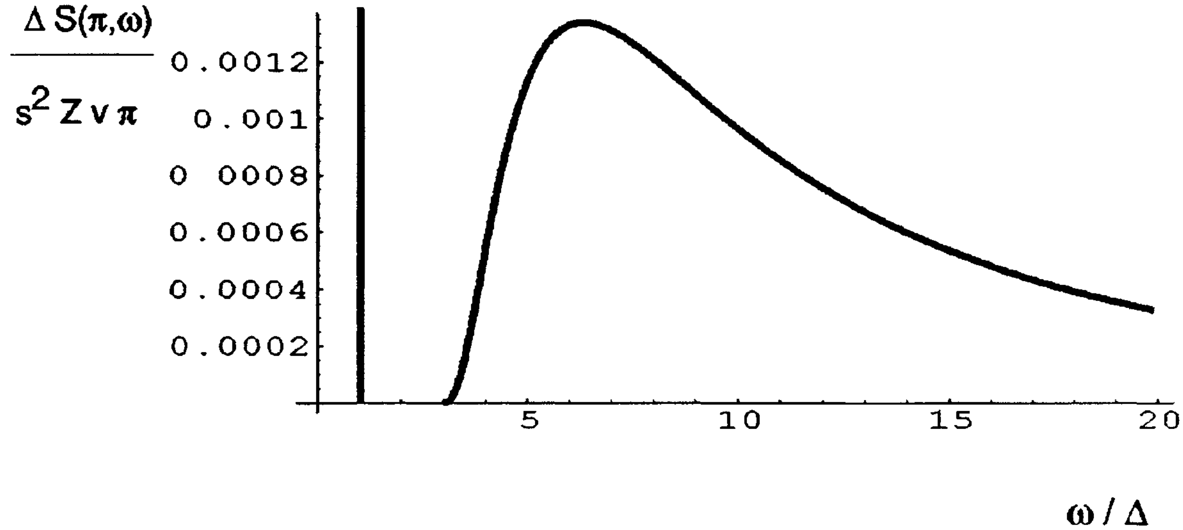
Note that at $n\to\infty$ we obtain the free-boson resul $G(\theta)=1$. Evaluating the integral for $n=3$, gives

$$G(\theta)=\frac{\pi}{4}\frac{\Gamma(\frac{1}{2}-\frac{i\theta}{2\pi})\Gamma(\frac{3}{2}+\frac{i\theta}{2\pi})}{\Gamma(1-\frac{i\theta}{2\pi})\Gamma(2+\frac{i\theta}{2\pi})}, \quad (3.9$$

where $\Gamma(z)$ is Euler's gamma function. Thus

$$|G(\theta)|^2=\frac{\pi^4}{64}\frac{1+(\theta/\pi)^2}{1+(\theta/2\pi)^2}\left(\frac{\tanh\theta/2}{\theta/2}\right)^2. \quad (3.1$$

At small θ this behaves as: $|G(\theta)|^2\approx 1.52(1-0.09\theta^2$



π ω σ

π

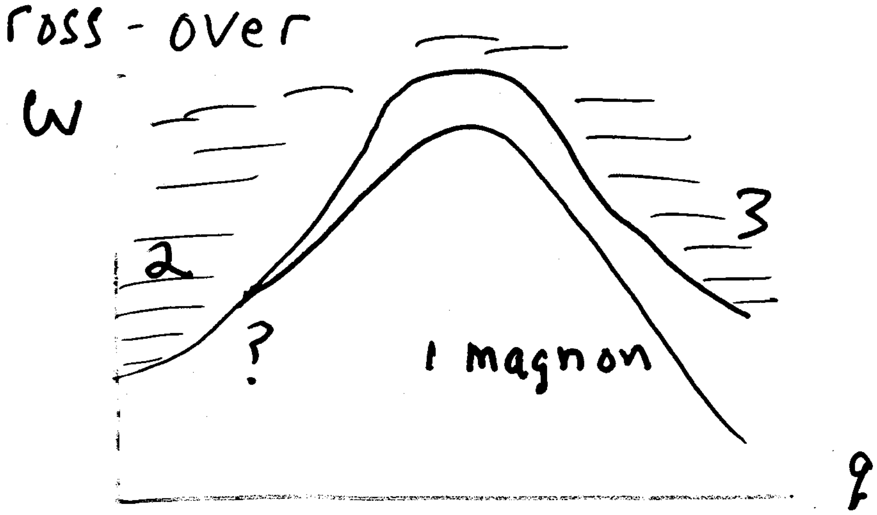
ω

π ω

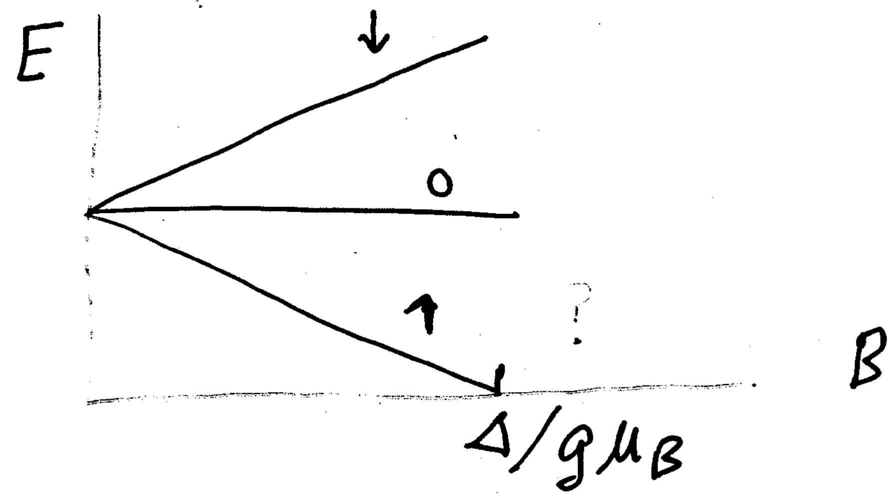
$$\frac{\pi}{\omega} \qquad \frac{\theta \quad \theta \quad \theta \quad \theta}{\pi}$$

$$\delta \quad \overline{\omega} \qquad \theta \quad \theta \quad \theta \quad -$$

another interesting problem, inaccessible to our low energy field theory approximation, is 2 magnon – 1 magnon cross-over



Magnetic Field Effects



- at critical field gap closes for spin-up magnons

- we may ignore (integrate out) spin 0, ↓ magnons
- since $\sum_j S_j^z$ commutes with H and since this operator is just total number of spin-up magnons (ignoring spin down and zero) it follows that B corresponds to chemical potential for spin-up magnons and phase transition is one-dimensional <u>Bose condensation</u>
- short-range repulsive interaction between (spin-up) magnons controls how density (i.e. magnetization) varies with B

Lagrangian becomes:

$$\mathcal{L} = \frac{1}{2}\left(\frac{\partial \vec{\varphi}}{\partial t} + \vec{B}\times\vec{\varphi}\right)^2 + \cdots$$

for $\vec{B} \parallel \hat{z}$, let $\psi \equiv (\varphi_1 - i\varphi_2)/\sqrt{2}$

$$\mathcal{L} = \left|\left(\frac{\partial}{\partial t} - iB\right)\psi\right|^2 + \cdots$$

$$\approx iB\left(\psi^\dagger \frac{\partial \psi}{\partial t} - \frac{\partial \psi^\dagger}{\partial t}\psi\right) + B^2|\psi|^2 + \cdots$$

- ψ is boson annihilation operator

$\mathcal{L}$ now takes essentially standard form for non-relativistic bosons

- although detailed form of boson interaction isn't known exactly many properties of Bose condensation are universal in $D=1$
- universality occurs when bosons are dilute so average separation $\frac{1}{\rho} \gg \xi$ (interaction range)

$$H_{eff} = -\frac{1}{2m}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_j^2} + \sum_{i\neq j} V(|x_i - x_j|)$$

- in dilute limit ground state is:

$\Psi_B(x_1 \ldots x_N) = \epsilon(x_1 \ldots x_N)\,\Psi_F(x_1 \ldots x_N)$

where ϵ is anti-symmetric step function ($= \pm 1$) and Ψ_F is <u>free fermion</u> (Bloch) wave-function

1) eigenstate of kinetic energy

2) $\Psi_B = 0$ when 2 bosons overlap

- i.e. any short-range interaction is like hard-core case at low density

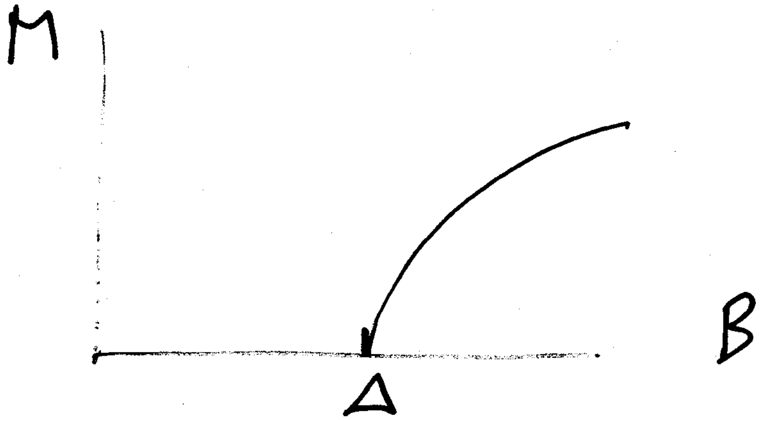
- we can now calculate $M(B)$ by pretending we have fermions:

$$\frac{M}{L} = \rho = \int_{-k_F}^{k_F}\frac{dk}{2\pi} = \frac{k_F}{\pi}$$

$$\frac{E}{L} = (\Delta - B)\rho + \int_{-k_F}^{k_F}\frac{dk}{2\pi}\,\frac{k^2}{2m} = (\Delta - B)\rho + \frac{\pi^2\rho^3}{6m}$$

- note that details of interactions don't enter although they are crucial!
- minimizing $E(\rho)$ gives:

$$\frac{M}{L} = \rho = \frac{1}{\pi v}\sqrt{2\Delta(B-\Delta)} \quad [\text{using } \Delta = mv^2]$$



above B_c low energy excitations are phonons in Bose condensate, corresponding to phase of ψ - i.e. magnons near $q = \pi$

$$\psi_B(x) \sim \sqrt{\rho_0}\, e^{i\varphi(x)/R}$$

$\varphi(x)$ is a free massless boson field.

- R-parameter can be fixed in dilute limit

- use relation to free fermions
- Jordan-Wigner transformation to fermion operator:

$$\psi_F(x) \sim e^{i\pi \int_{-\infty}^{x} \rho(y)dy} \psi_B(x)$$

$\psi_F(x)$ should have scaling dimension 1/2 corresponding to free fermions in dilute limit

$$\rho(x) \sim \rho_0 + \frac{1}{R}\frac{\partial \varphi}{\partial t} \quad [\text{so } [\rho(x), \psi_B(y)] = \delta(x-y)\psi_B(x)]$$

$$\psi_F \sim e^{i\rho_0 x} e^{i\left[\frac{\varphi}{R} + R\int^{x}\frac{\partial \varphi}{\partial t}\right]}$$

- this gives bosonized expression for free fermion field if $R = 1/\sqrt{\pi}$ $\Rightarrow$

$$\langle S^+_j S^-_0 \rangle \sim \frac{(-1)^j}{|j|^{1/2}}$$

next correction to $M(\beta)$ depends on details of interactions only through scattering length of effective interaction

i.e. consider symmetric 2-particle wave-function:

$$\psi(x) \to \sin[q|x| + \delta(q)] \quad (|x| \gg \xi)$$

$$\delta(q) \to -aq \quad (q \to 0)$$

- defines scattering length a
- N-particle wave-function in next approximation can be constructed following exact sol'n of δ-function case:

$$\psi(x_1, \ldots x_N) = \sum_P A(P)\, P \exp\left[i \sum_{j=1}^{N} q_j x_j\right]$$

- here P permutes the momenta, q,
- from considering what happens when

when 2 particles come close together:

$$A(Q) = -A(P)\, e^{i 2\delta\left[\frac{q_i - q_j}{2}\right]}$$

where permutations P, Q differ only by interchanging $q_i \leftrightarrow q_j$

- periodic boundary conditions then determine the q_j by:

$$(-1)^{N-1} e^{-i q_j L} = \exp\left[i \sum_{s=1}^{N} 2\delta\left(\frac{q_s - q_j}{2}\right)\right]$$

- for δ-fnc. gas this is exact since 3 particles never interact simultaneously
- for general short-range potential this gives leading low density behavior
- since q_j are all small, this becomes:

$$q_j (L - Na) + a \sum_s q_s = \pi n_j, \quad (\text{for all } j)$$

- here n_j is even (N odd) or odd (N even)

$$k_j \simeq \frac{\pi n_j}{L} - \frac{a}{L} \sum_{s=1}^{N} (n_s - n_j) \frac{\pi}{L}$$

$$E = \frac{1}{2m} \sum k_j^2 \simeq \frac{1}{2m} \sum_{j=1}^{N} \left(\frac{\pi n_j}{L}\right)^2 + \frac{a}{2mL} \sum_{(i,j)} \left[\frac{\pi (n_i - n_j)}{L}\right]$$

- a convenient way to determine a numerically for spin-1 chain is to calculate E for N = 2 and fit $1/L^2$, $1/L^3$ terms $\Rightarrow$

$a \simeq -.34\,\xi \qquad [\xi = 6.03]$

- for NLσM exact 2-body S-matrix is known - gives $\delta(q)$ and hence scattering length:

$a_{NL\sigma M} = -\frac{2}{\pi}\xi$ [agreement with S=1 chain is poor]

magnetization can now be expressed in terms of a:

$$\frac{M}{L} = \frac{1}{\pi V}\left[\sqrt{2\Delta(\beta-\Delta)} - \frac{\delta a \Delta}{3\pi V}(\beta-\Delta) + \cdots\right]$$

(expansion in $a\rho$)

- this can be extended easily to finite T (Fermi distribution function)
- can also be extended to finite L paying care attention to parity of n_j's depending on number of magnons [gives imaginary term in chemical potential:

$$(-1)^N = \exp\left[i\pi \sum_j n_j\right]\Big]$$

- agreement with Monte Carlo for $L = \frac{1}{T} = 100$ is surprisingly good
- a number of other effects must be accounted for to fit experiments

in particular, interchain couplings, which are not too important at $B=0$ in highly 1D compounds ($J'/J < .01$) produce Néel order above B_c

Conclusions

- no gap for $S=\frac{1}{2}$, gap for $S=1$
- free massless boson gives <u>exact</u> $E \to 0$ behavior in gapless case
- massive NLσM gives <u>qualitative</u> behavior for $S=1$
- staggered field opens gap for $S=\frac{1}{2}$
  - massive sine-Gordon model
- uniform field closes gap for $S=1$
  - Bose condensation

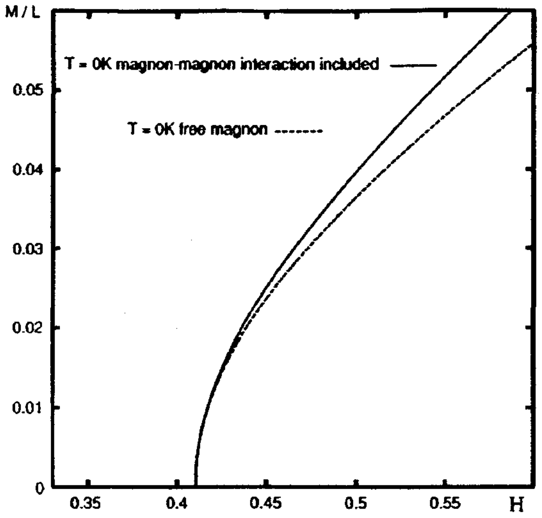


FIG. 7. Magnetization curve for $S=1$ chain near critical field $H_c=\Delta$. (The exchange constant and $g\mu_B$ are set equal to 1.) For infinite length and at $T=0$, we plot it as given in Eq. (4.7). The full line has included the leading-order contribution of magnon-magnon interactions. The dashed line is a reference line for comparison and it is for free hard-core boson approximation.

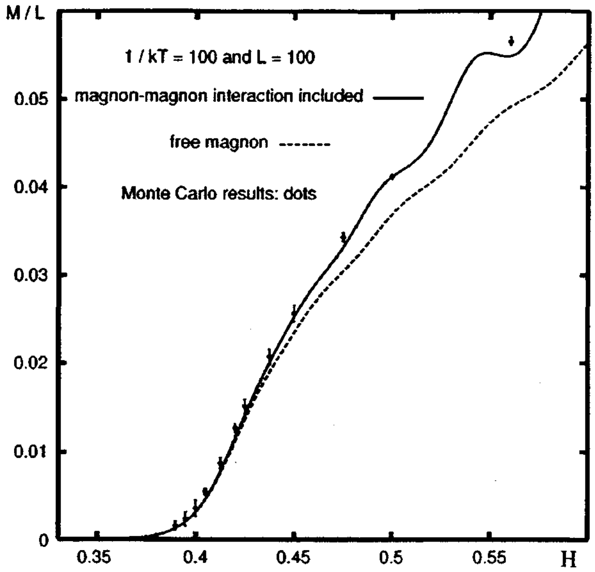


FIG. 8. Magnetization curve for $S=1$ chain near critical field $H_c=\Delta$, with length $L=100$ and at temperature $kT=1/100$. The full line has included the leading-order contribution of magnon-magnon interaction. The dashed line is a reference line for comparison and it is for the free hard-core boson approximation. The dots are the Monte Carlo results (Ref. 19).

$$E_0(n)/L=(\Delta-H)n+\int_{-k_F}^{k_F}\frac{dk}{2\pi}\frac{k^2}{2m}+\frac{a}{2m}\int_{-k_F}^{k_F}\frac{dk}{2\pi}\int_{-k_F}^{k_F}\frac{dk'}{2\pi}(k-k')^2. \quad (4.5)$$

Here we have included the Zeeman term, $-Hn$ in the energy; H is the applied magnetic field. Performing the integrals gives

$$E_0(n)/L=(\Delta-H)n+\frac{\pi^2n^3}{6m}+\frac{a\pi^2n^4}{3m}. \quad (4.6)$$

This represents an expansion of the energy in powers of the density. The first term which depends on the interactions is the $O(n^4)$ term. Minimizing E_0 with respect to n gives the density or magnetization per unit length:

$$M(H)/L=n\approx\frac{1}{\pi v}\left[\sqrt{2\Delta(H-\Delta)}-\frac{8a\Delta}{3\pi v}(H-\Delta)\right]. \quad (4.7)$$

In Fig. 7 we plot M/L vs H from Eq. (4.7) with and without the interaction ($a=-0.34\xi$ or $a=0$). The leading-order correction due to the magnon-magnon interaction is obvious around magnetization $M/L=0.02$.

This finite density correction can be generalized to finite temperature T, as was observed by Okunishi[26] in the special case of the δ-function interaction. The correction to the free energy of lowest order in density is given by including thermal occupation numbers in the second term of Eq. (4.5):

$$\Delta F/L=\frac{a}{2m}\int\frac{dk_1dk_2}{4\pi^2}n_F(k_1)n_F(k_2)(k_1-k_2)^2. \quad (4.8)$$

Note that it is the *Fermi* distribution function which appears, rather than the Bose function. This simply follows from the condition that the k_j should all be distinct so that there is an effective occupation number for each momentum which can be 0 or 1 only. $n_F(k)$ is evaluated at finite T and H, then the magnetization is obtained by the usual thermodynamic formula, $\partial F/\partial H=-M$. In order to compare with recent Monte Carlo data on the magnetization for the $S=1$ chain, it is useful to also generalize our formulas to finite length, L with periodic boundary conditions. There is a slight subtlety in doing so because the allowed wave vectors of the magnons alternate between $k=2\pi n/L$ ("even wave vectors") for an odd number of magnons and $k=2\pi(n+1/2)/L$ ("odd wave vectors") for an even number. This follows from the sign change of the wave function each time one magnon passes another one. However, this is easily dealt with exactly by inserting appropriate factors of

$$(-1)^N=e^{i\pi\sum_k n_k}, \quad (4.9)$$

into the partition function trace. This effectively gives the chemical potential an imaginary part, essentially converting fermion occupation numbers into boson ones. For $a=0$, the partition function is given by

$$Z^0=(1/2)[Z^0_{Fe}-1/Z^0_{Be}+Z^0_{Fo}+1/Z^0_{Bo}]. \quad (4.10)$$

Here Z^0_{Fe} denotes the partition function for free fermions with even wave vectors; Z^0_{Bo} denotes the partition function for bosons with odd wave vectors, etc. Note that *inverse* boson partition functions occur. The thermal average of the second term in Eq. (4.3) becomes