BEYOND THE TOMONAGA-LUTTINGER MODEL: Dynamical critical behaviour of the xxz spin chain

with

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1^{ST} LECTURE-small q

- Introduction
- Band curvature effects at small q
- Effective Hamiltonian – exact coupling constants
- Exact results for high energy tail of $S(q,\omega)$
- Behaviour near peak of $S(q,\omega)$
- Bethe ansatz and Density Matrix Renormalization group (DMRG) results

OUTLINE-2nd LECTURE

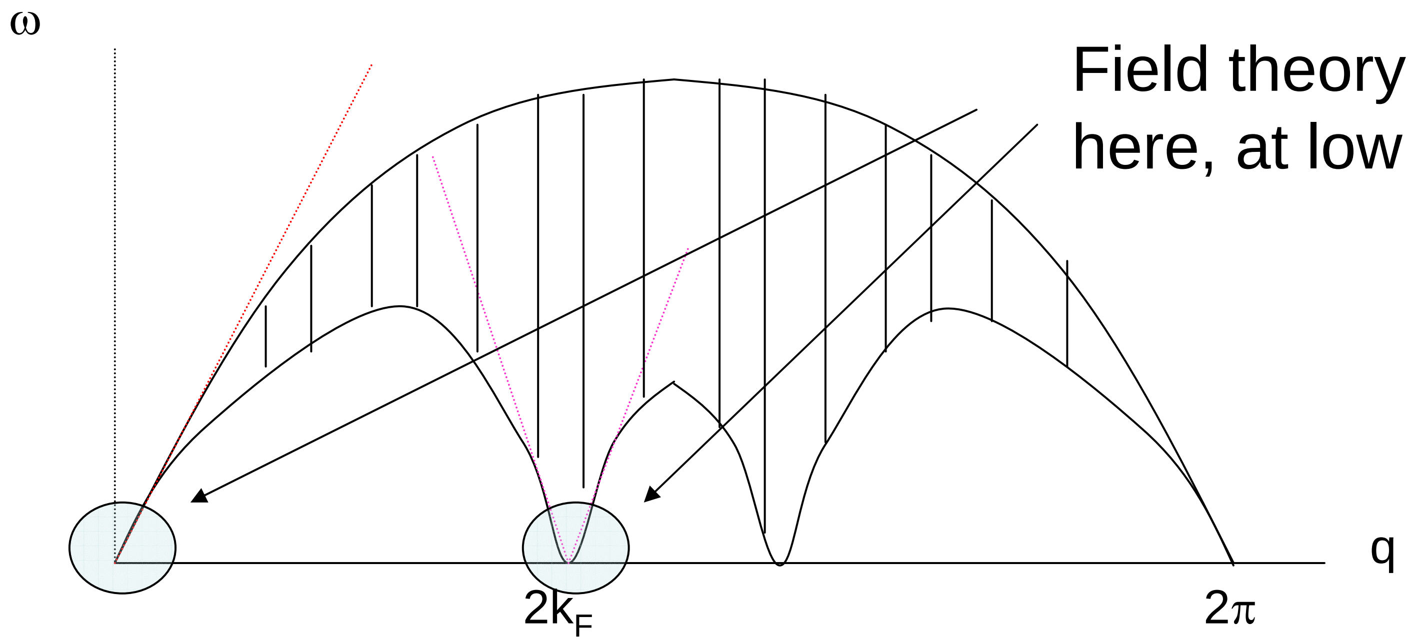
- “X-ray edge” field theory methods
- Finite size spectrum and Bethe Ansatz
- Long time behaviour of self-correlation function
- Comparison to Dynamical Density Matrix Renormalization Group results
- Open questions

Introduction

$$H = \sum_{j=1}^{N} [S_j^x \cdot S_{j+1}^x + S_j^y \cdot S_{j+1}^y + \Delta S_j^z \cdot S_{j+1}^z - h S_j^z],$$

$$|\Delta| < 1, \;\; h < h_S, \;\; \vec{S}_{N+1} = \vec{S}_1$$

$$S(q,\omega) = \frac{1}{N} \sum_{j,j'=1}^{N} e^{-iq(j-j')} \int_{-\infty}^{\infty} dt \, e^{i\omega t} < 0 | S_j^z(t) S_{j'}^z(0) | 0 >$$

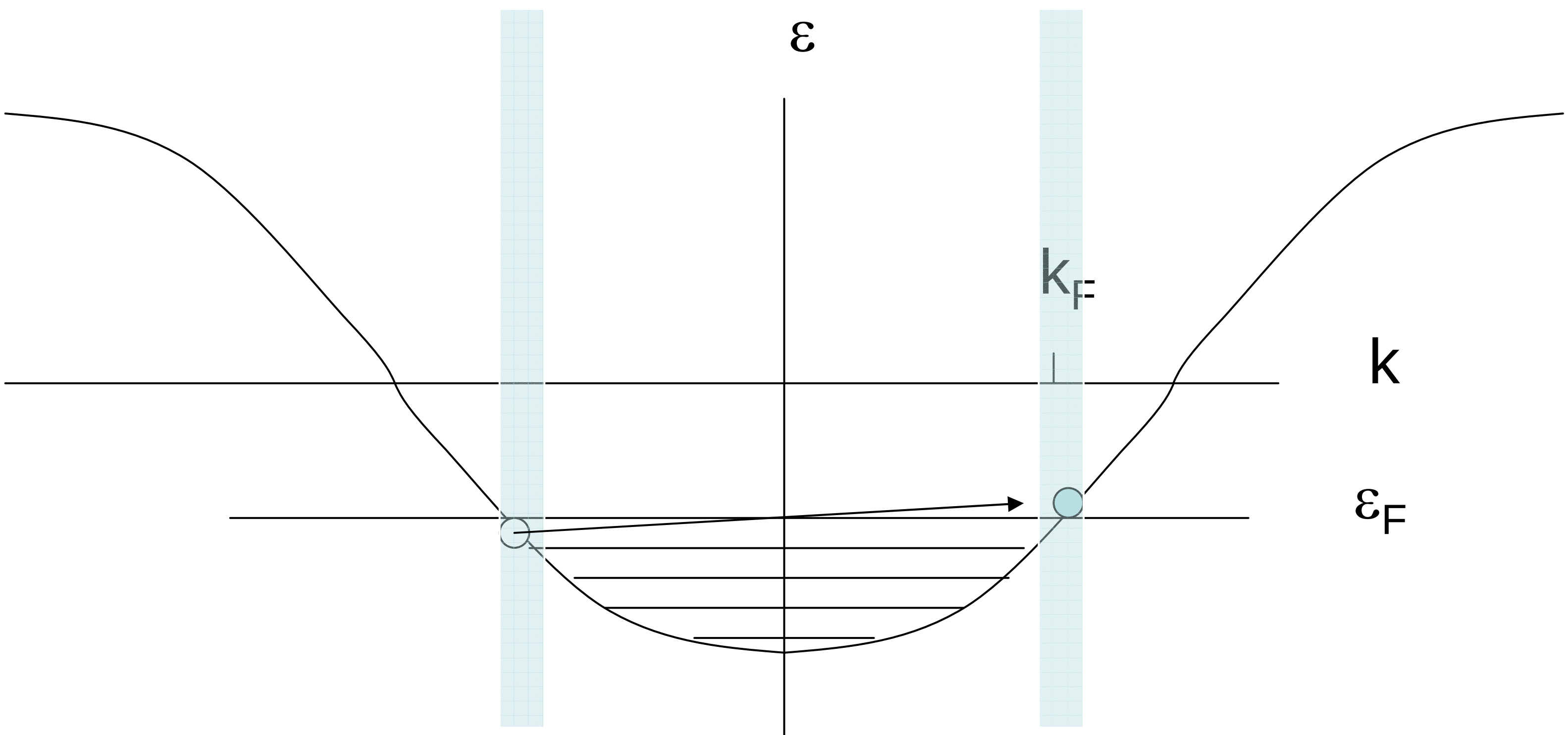


Field theory works <u>only</u> here, at low ω??

Jordan-Wigner transformation:

$$H = \sum_{j=1}^{N} [-\tfrac{1}{2}(c_j^+ c_{j+1} + h.c.) + \Delta n_j n_{j+1}]$$

$$c_j \approx e^{ik_F j}\psi_R(j) + e^{-ik_F j}\psi_L(j)$$



Low energy q≅2k_F excitation

Linearizing the fermion dispersion relation and bosonizing gives:

$$S_j^z \approx (\psi_L^+\psi_L + \psi_R^+\psi_R) + (e^{2ik_F j}\psi_L^+\psi_R + e^{-2ik_F j}\psi_R^+\psi_L)$$
$$\approx \sqrt{\frac{K}{\pi}}\partial_x\phi + \text{const}\cdot\cos[\sqrt{4\pi K}\phi + 2k_F j]$$
$$\psi_{R/L} \propto \exp[i(-\sqrt{\pi K}\theta \pm \sqrt{\pi / K}\phi)]$$

With an effective free boson Hamiltonian density:

$$H = \frac{1}{2v}\Pi^2 + \frac{v}{2}(\partial_x\phi)^2$$

- The velocity, v, and Luttinger parameter, K, can be determined from Bethe ansatz results
- We can obtain low energy S(q,ω) and fermion Green's functions in terms of free boson Green's functions

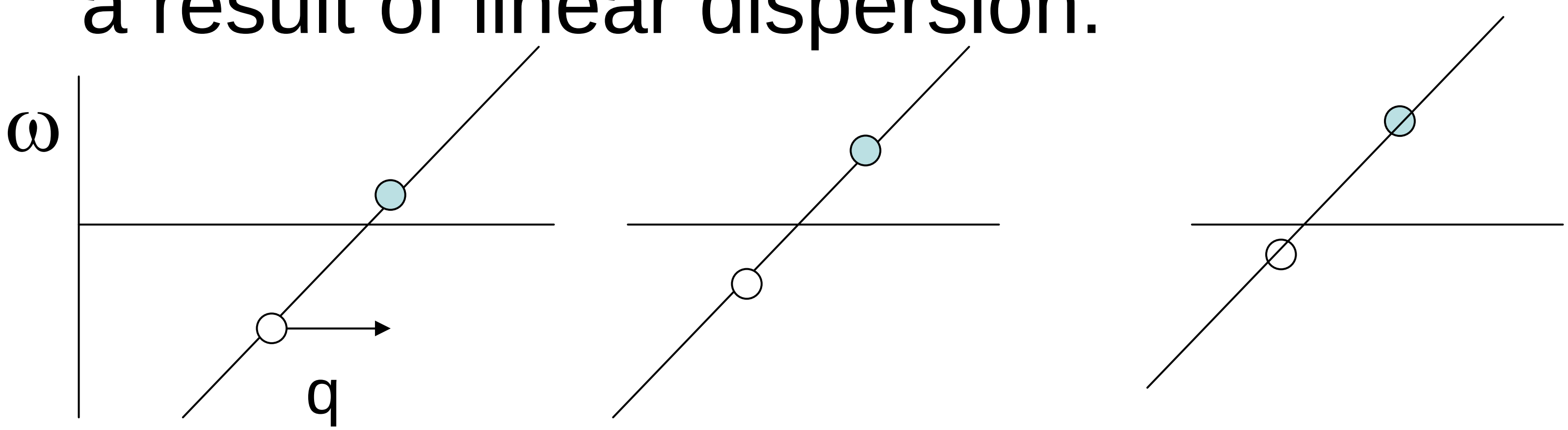
BAND CURVATURE EFFECTS

- At small q, Luttinger liquid theory predicts

$S^{zz}(q,\omega)=(K/\pi)<\partial_x\phi\ \partial_x\phi>=Kq\delta(\omega-v|q|)$

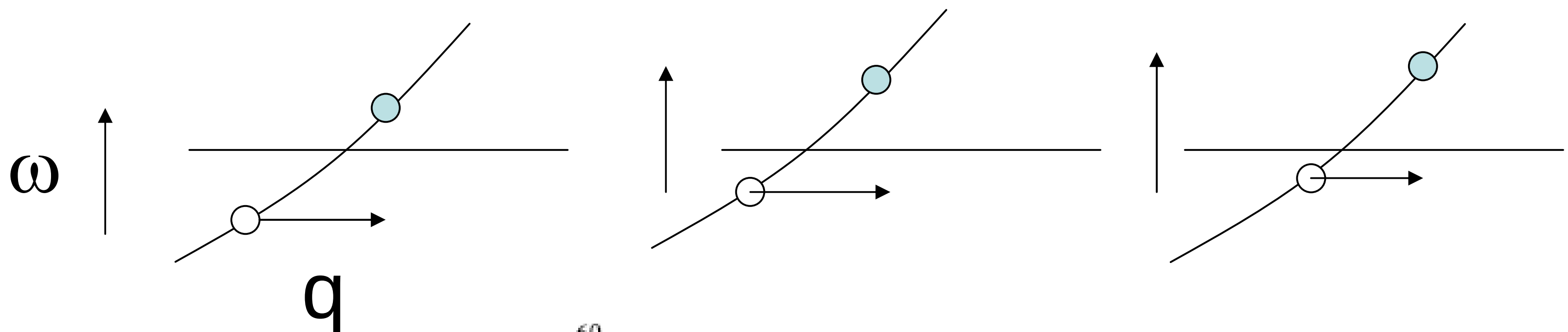
- In free fermion case this simple form is

a result of linear dispersion:

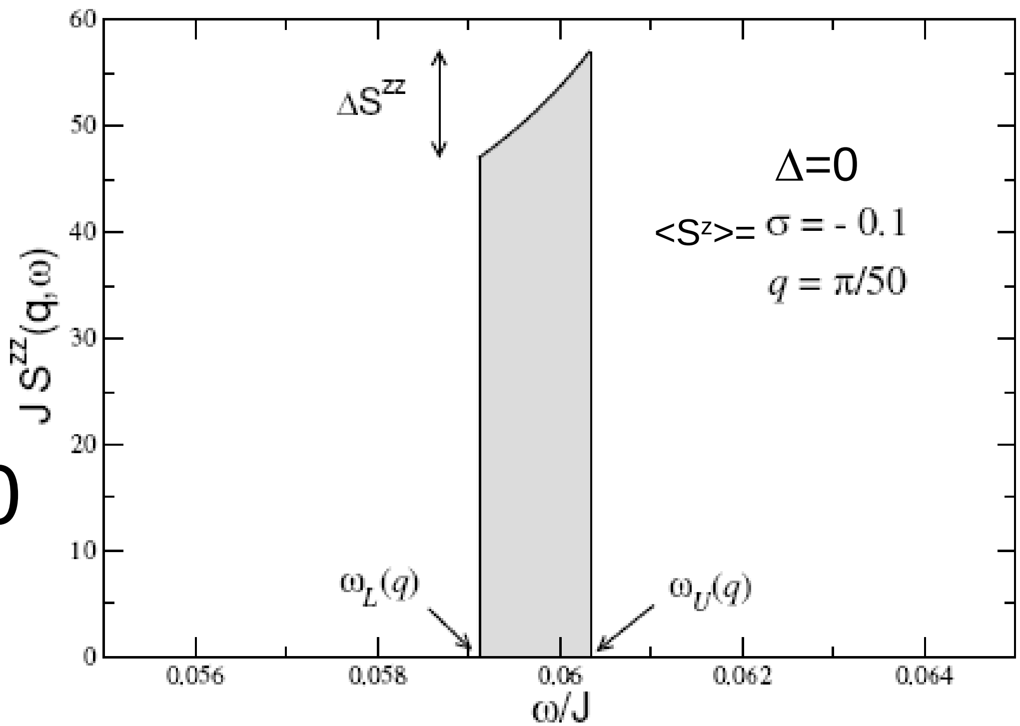


All particle-hole excitations of wave-vector q have same energy, $\omega=v|q|$

Including band curvature gives finite width:



width, $\Delta\omega \sim q^2$
so LL theory
is almost
correct as $q \Rightarrow 0$



- What happens if we include both band curvature *and* interactions ($\Delta \neq 0$)?
- Does width still scale as q^2?
- What is line shape?
- Could steps turn into power law divergences?
- Can we study these questions with field theory techniques?
- What information can we extract about these questions from Bethe ansatz solution?
- What can we learn from numerical techniques (Density Matrix Renormalization Group)?

EFFECTIVE HAMILTONIAN: EXACT COUPLING CONSTANTS

- Band curvature gives interactions upon bosonizing even for Δ=0!

$$\psi_L^{+}\partial^2\psi_L \approx \frac{\sqrt{2\pi}}{3}\left(\partial_x\phi_L\right)^3$$

- Interactions in lattice model given another cubic term. Including both:

$$\delta H = \frac{\sqrt{2\pi}}{6}\int dx\,\left\{\eta_-\left[\left(\partial_x\varphi_L\right)^3-\left(\partial_x\varphi_R\right)^3\right]+\eta_+\left[\left(\partial_x\varphi_L\right)^2\partial_x\varphi_R-\left(\partial_x\varphi_R\right)^2\partial_x\varphi_L\right]\right\}$$

- These are most general dimension 3 interactions allowed by parity
- They destroy Lorentz invariance and particle-hole symmetry ($\varphi\rightarrow-\varphi$)

•We may derive exact identities relating $\eta_\pm$ to derivatives of Luttinger parameter and velocity with respect to field, h:

$$J\eta_- = \frac{v}{K^{1/2}}\frac{\partial v}{\partial h} + \frac{v^2}{2K^{3/2}}\frac{\partial K}{\partial h}$$

$$J\eta_+ = \frac{3v^2}{2K^{3/2}}\frac{\partial K}{\partial h}.$$

•v(h) and K(h) can be determined to high accuracy from numerical solution of thermodynamic Bethe ansatz equations

•Thus coupling constants, $\eta_\pm$ can be determined essentially exactly

BEHAVIOUR NEAR TAIL OF S

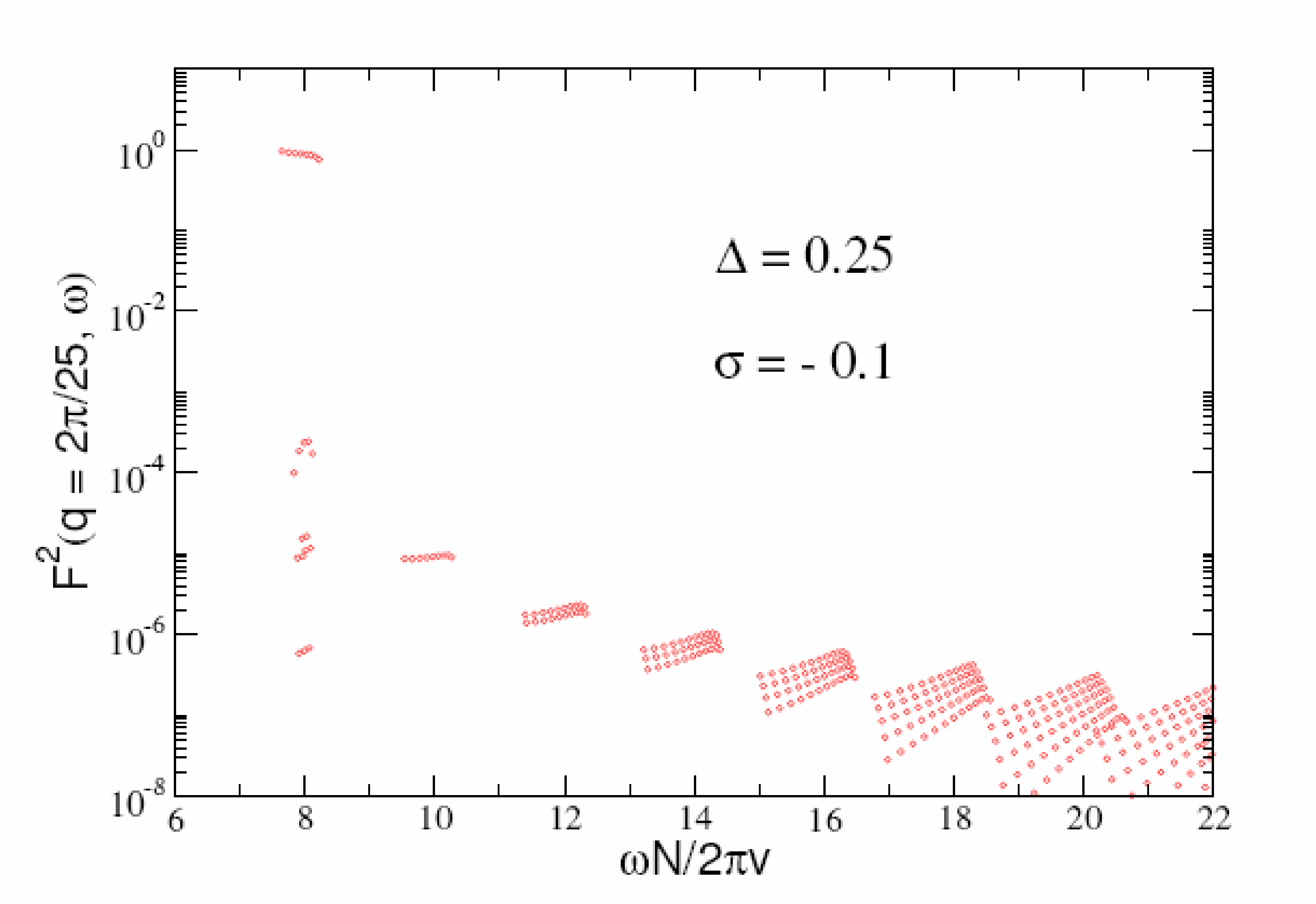
- Lowest order perturbation theory in $\eta_{\pm}$ gives retarded Green's function:

$$S = Kq\delta(\omega - v|q|) + \eta_-^2 \frac{Kq^5}{24}\frac{d^2}{d\omega^2}\delta(\omega - v|q|) + \eta_+^2 \frac{Kq^4\theta(\omega - v|q|)}{18v(\omega^2 - v^2q^2)} + \dots$$

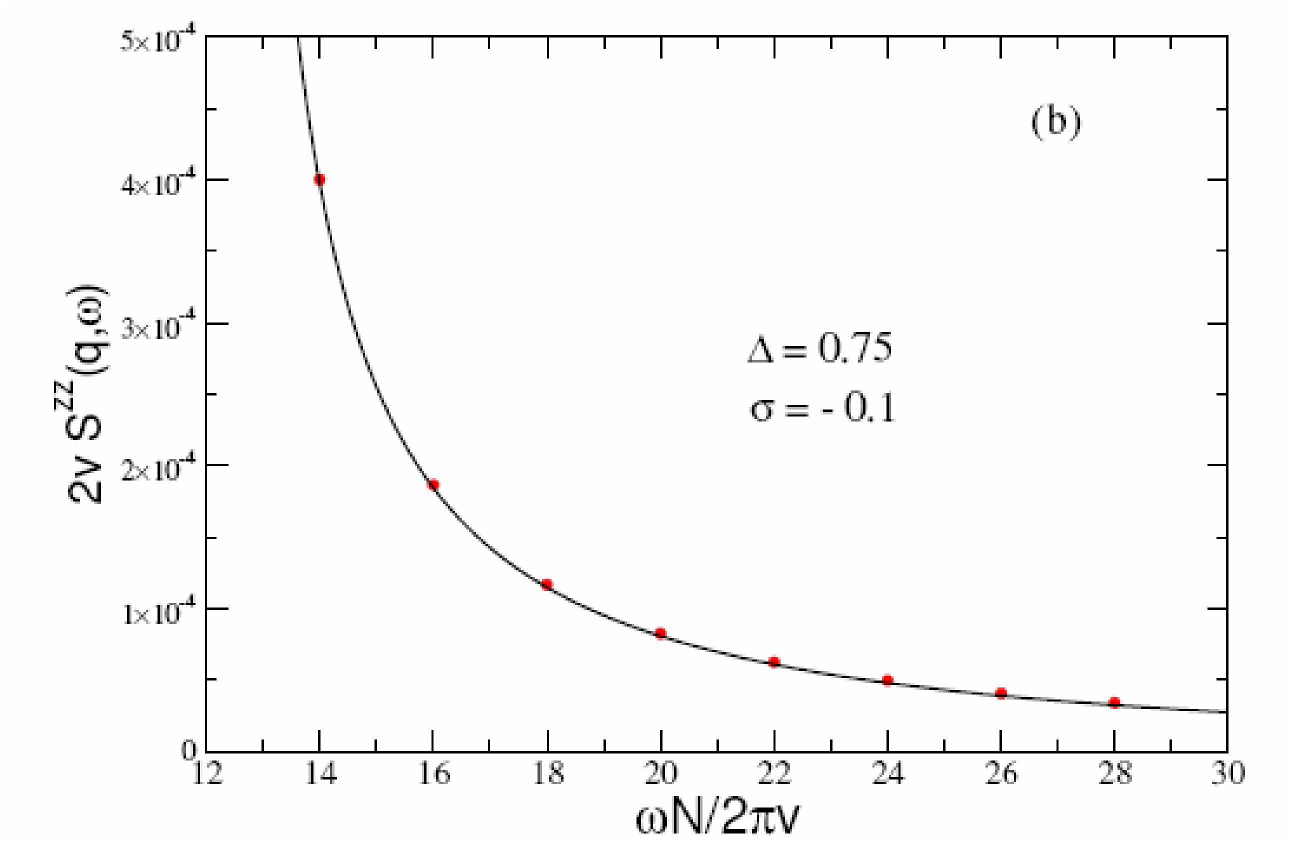
•Note that, while both corrections are suppressed by 2 extra power of q or ω, they diverge "on mass shell" near ω~v|q|

•We can only trust this perturbation theory far from mass shell: ω-v|q|>> $q^2\eta_{\pm}$

- η_+^2 term predicts a “high energy tail” for S
- We compared this to Bethe ansatz:
- Up to 2000 form factors were calculated:
- $<0|S^z(q)|n>$, 2-particle, … up to 8-particle for finite length chains up to length N=600
- We extend the field theory result to finite N by the usual conformal transformation
- Field theory predicts states at discrete energies: $\omega=2\pi vn/N$, n=1,2,3,… whereas Bethe ansatz states are scattered
- We bin BA states to make comparison:



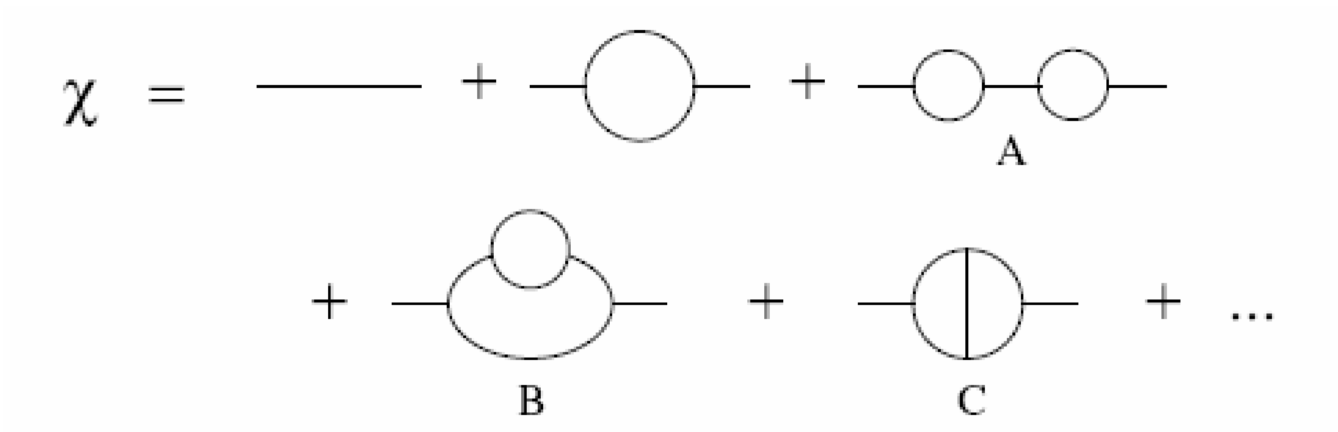
Bethe ansatz squared form factors



- Red dots are BA results, line is field theory
- Note that we have no adjustable parameters (all fixed from thermodynamic BA) and we are at strong coupling

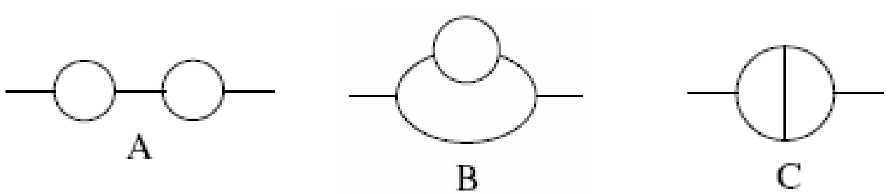
BEHAVIOUR NEAR PEAK

- We need to somehow sum series in $\eta_{\pm}$ to get sensible result near peak
- We explicitly calculated series in η_{-} to 4^{th} order:



$$\chi(q, i\omega) = \frac{Kq}{2\pi w}\left[1 + \frac{1}{3}\left(\frac{\eta\_q^2}{2w}\right)^2 + \frac{1}{5}\left(\frac{\eta\_q^2}{2w}\right)^4 + \dots\right]$$

Here $w \equiv i\omega - vq$ and the 4^{th} order term gets contributions from all 3 diagrams:
$1/[5 \times 2^4] = 1/144 + 1/504 + 1/280$



•Tells us that no simple partial resummation (RPA, SCBA,…) will be sufficient!

• Series in η_- should sum up to give free fermion result, including band curvature at small q

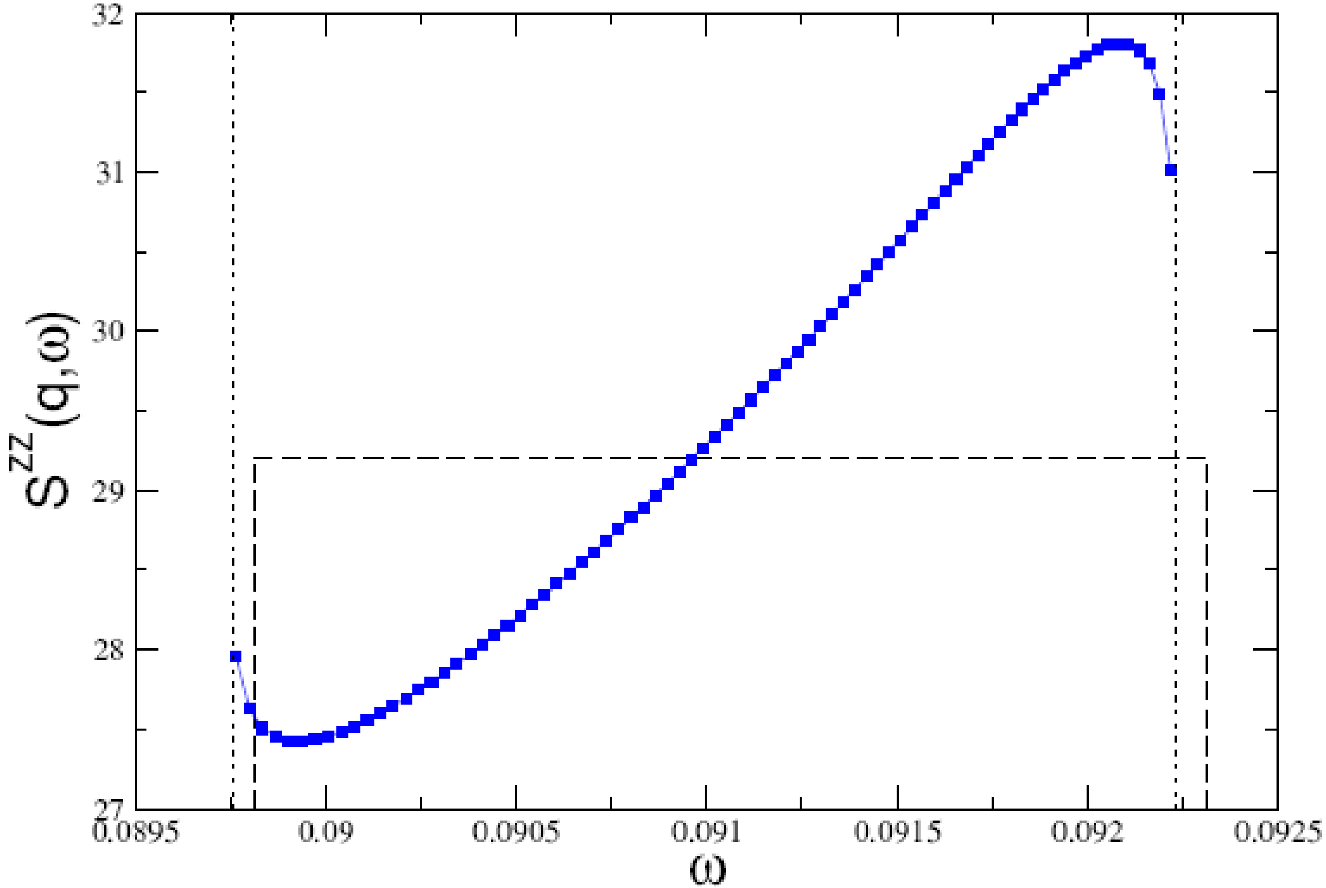
$$\chi(q, i\omega) = \frac{K}{2\pi\eta_- q} \log\left[\frac{i\omega - vq + \eta_- q^2/2}{i\omega - vq - \eta_- q^2/2}\right]$$

Implying:

$$S^{zz}(q, \omega) = \frac{K}{\eta_- q}\theta\left(\frac{\eta_- q^2}{2} - |\omega - vq|\right)$$

but we have no idea how to sum η_+ terms

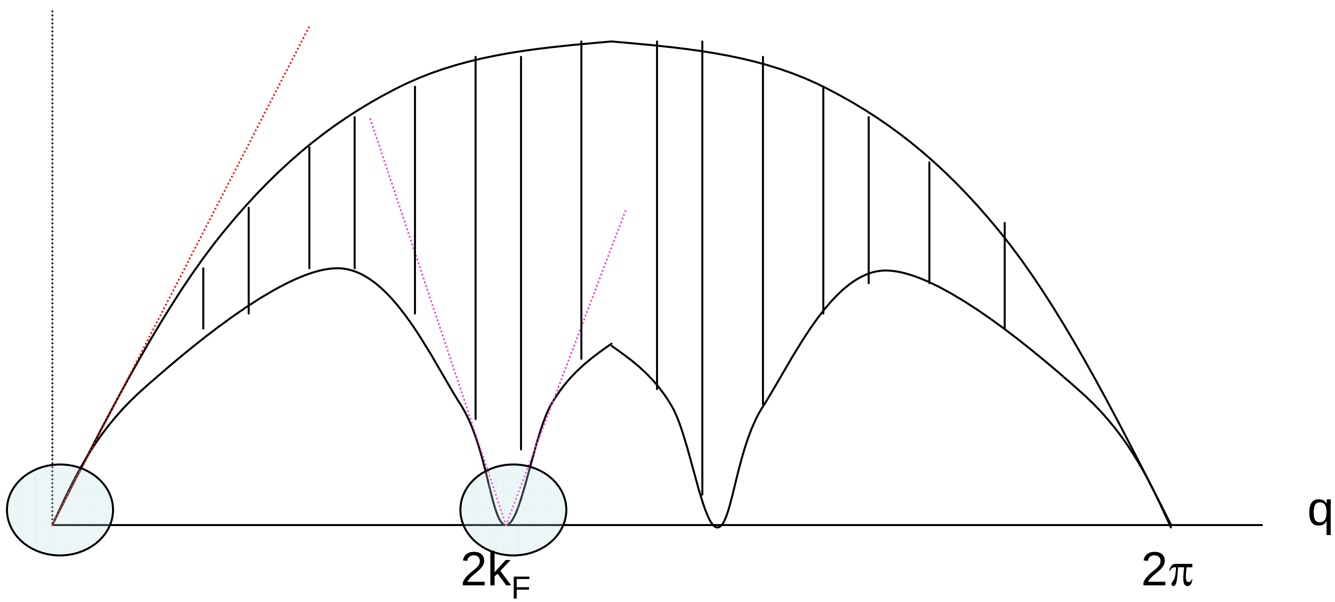
This crude (η_- only) approximation, seems to give correct line-width, $\sim q^2$ and height but misses line shape and power law singularities



Δ=.25
σ=-.1
N=6000

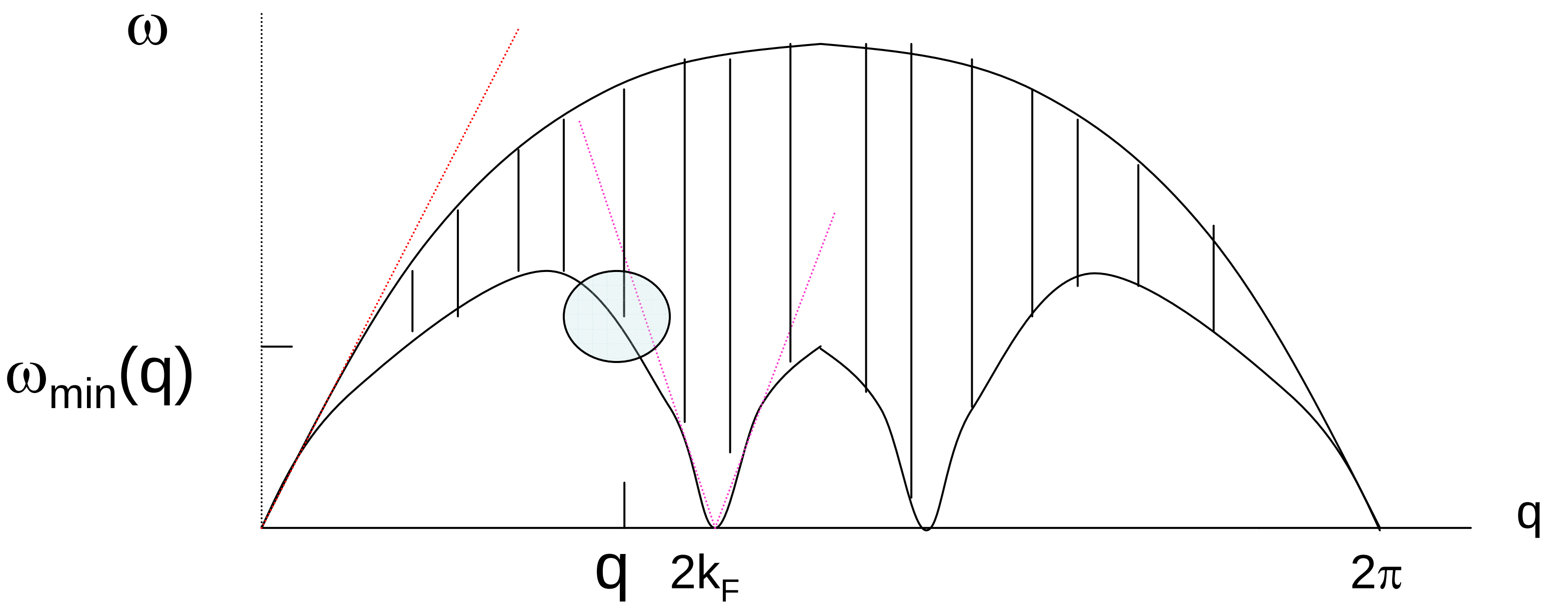
- Blue dots are BA results (2 particle states only)
- Dashed line is field theory result ignoring η_+

- We can't get enough resolution from finite size BA, with limited number of states kept, to study singularities
- We don't know how to sum series in η_+ to make field theory predictions for singularities
- Singularities may also exist at q of O(1) – we would like to study those also

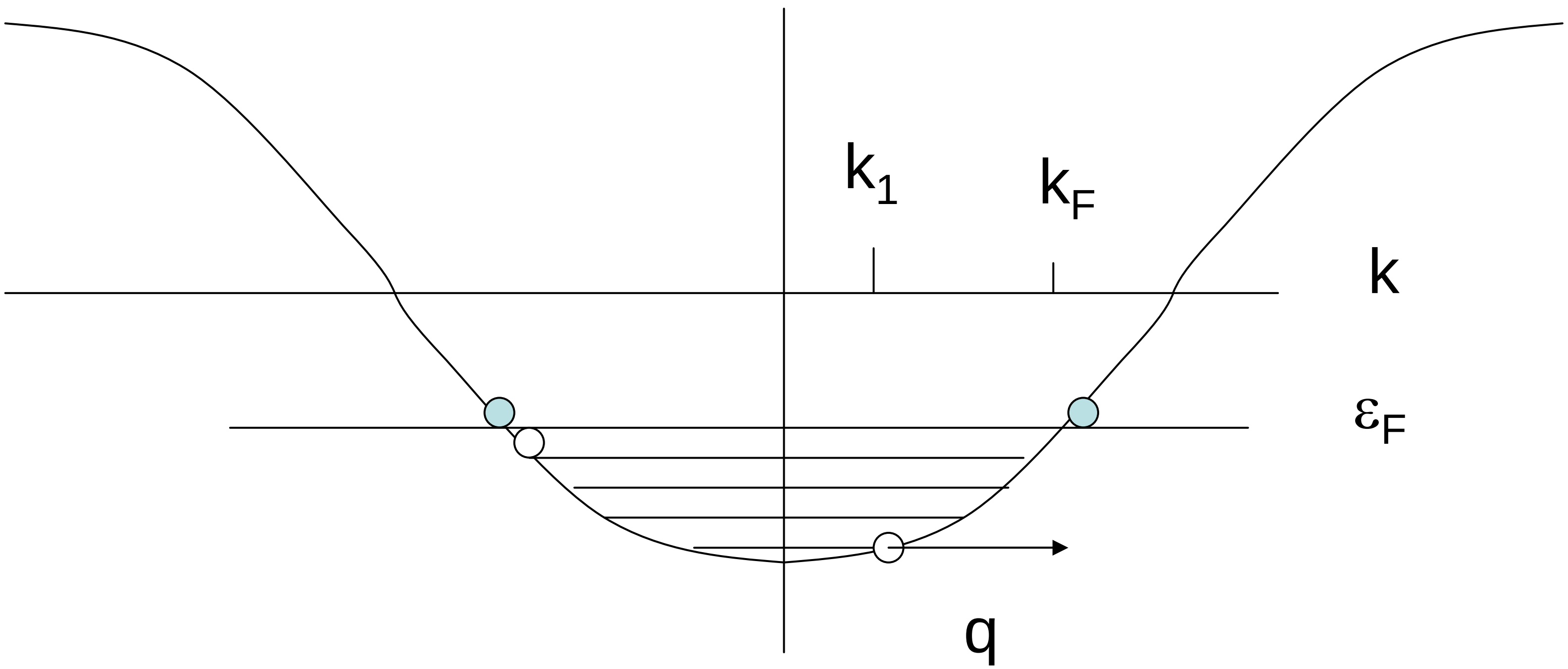


X-Ray Edge Field Theory Methods

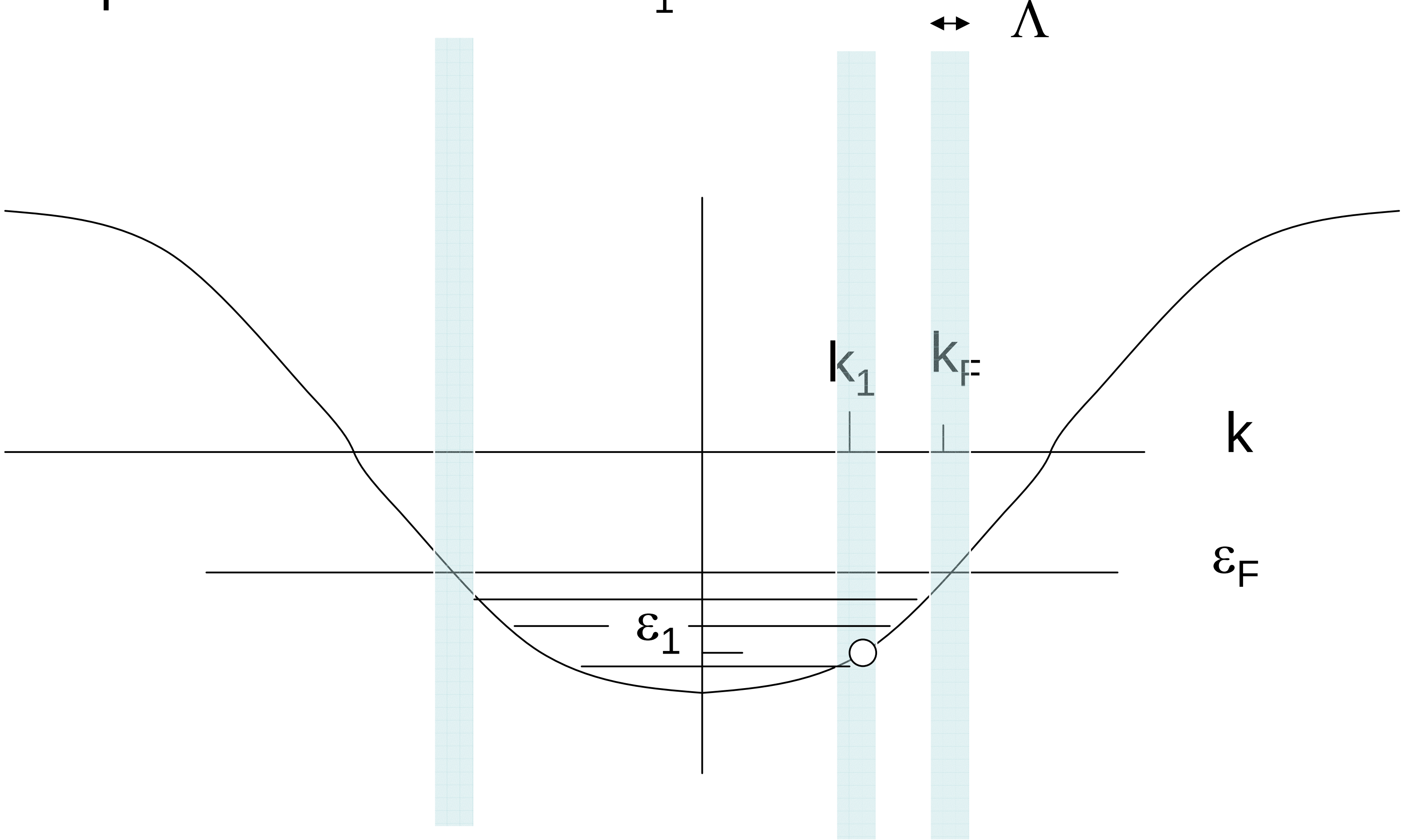
We can calculate $S(q,\omega)$ near ω_{min} (q) *for any q* using other field theory techniques first developed for study of X-ray edge singularities – Pustilnik, Glazman, …



- Consider excitations with one “deep hole” at k_1 and many particles and holes near $\pm k_F$
- These appear to give lower threshold for hole Green’s function at momentum k or of $S(q,\omega)$ at $q=\pm k_F - k_1$



To calculate $G_F(k_1,\omega)$ and $S(\pm k_F - k,\omega)$, we consider a "low energy" effective Hamiltonian, H_k, containing only Fourier modes of fermions near k and $\pm$ k_F for the particular value of $k=k_1$ of interest



$$c_j \approx e^{ik_F j}\psi_R(j) + e^{-ik_F j}\psi_L(j) + e^{ik_1 j} d(j)$$

$$H \approx H_{TLL} + d^+(\varepsilon_1 - iu_1\partial_x)d + (\tilde{\kappa}_L \psi_L^+ \psi_L + \tilde{\kappa}_R \psi_R^+ \psi_R) d^+ d$$

- N.B. we haven't included any terms that would allow the "heavy hole" to decay
- Validity of this is complicated and not completely understood
- Now looks like model for a single "heavy" hole interacting with a Tomonaga-Luttinger Liquid (see Tsukamoto, Fujii, Kawakami, PRL 100, 126403, 1998)
- Now we bosonize the fermions near the Fermi surface only:

$$H = \frac{1}{2v}\Pi^2 + \frac{v}{2}(\partial_x \phi)^2 + d^+(\varepsilon_1 - iu_1\partial_x)d$$

$$+ \frac{1}{\sqrt{2\pi K}}(\kappa_L \partial_x \phi_L + \kappa_R \partial_x \phi_R) d^+ d$$

- All parameters: ε_1, u_1, κ_L, κ_R, depend on our arbitrary choice of heavy hole momentum, k_1, and are renormalized by the interactions, as we integrate out all wave-vectors except for the 3 narrow bands near k_1, $\pm k_F$
- Nonetheless, we determine them exactly using Bethe Ansatz
- Once these parameters are known, we can calculate the edge exponents by making a unitary transformation:

$$U = \exp\left\{ -\frac{i}{\sqrt{2\pi K}} \int_{-\infty}^{\infty} dx \left[\gamma_R \phi_R + \gamma_L \phi_L \right] d^+ d \right\}$$

- The parameters $\gamma_{L/R}$ are chosen to eliminate the marginal interactions $\sim \partial_x \phi_{L/R} d^+ d$, leaving only irrelevant ones with 2 or more derivatives

$$\gamma_{L/R} = \frac{\kappa_{L/R}}{v \pm u_1}$$

The transformed Hamiltonian is just free fields:

$$H = \frac{1}{2v}\tilde{\Pi}^2 + \frac{v}{2}(\partial_x \tilde{\phi})^2 + \tilde{d}^+(\varepsilon_1 - iu_1\partial_x)\tilde{d}$$

But the fermion d-field now contains a boson factor:

$$d = \tilde{d}\exp\left[-\frac{i}{\sqrt{2\pi K}}(\gamma_R \tilde{\phi}_R + \gamma_L \tilde{\phi}_L)\right]$$

and thus: $$d^+\psi_R \prec \exp[-i\sqrt{2\pi\nu_+}\tilde{\phi}_R + i\sqrt{2\pi\nu_-}\tilde{\phi}_L]\tilde{d}^+$$

where: $$\sqrt{\nu_\pm} = \frac{1}{4}\left[\sqrt{K} \pm \frac{1}{\sqrt{K}}\left(1 - \frac{\gamma_{R/L}}{\pi}\right)\right]$$

and similarly for $d^+\psi_L$

•Fortunately, the free fermion Green's function has a very simple form:

$$< 0 | \tilde{d}^{+}(x,t)\tilde{d}(0,0) | 0 > \approx e^{-i\varepsilon_1 t}\int_{-\Lambda}^{\Lambda} dk\, e^{ik(x-u_1 t)} \approx e^{-i\varepsilon_1 t}\,\delta(x-u_1 t)$$

Thus, for example:

$$S(q,\omega) \propto \int_{-\infty}^{\infty} dt \frac{e^{i(\omega-\omega_L)t}}{[(v-u_1)t-i\delta]^{\nu_+}[(v+u_1)t-i\delta]^{\nu_-}}$$

where $\delta \to 0^+$

•N.B. if $v>u_1$, this vanishes for $\omega<\omega_L$, as expected for a *lower* edge singularity:

$$S(q,\omega \sim \omega_L) \propto \theta[\omega-\omega_L(q)][\omega-\omega_L(q)]^{\nu_+ +\nu_- -1}$$

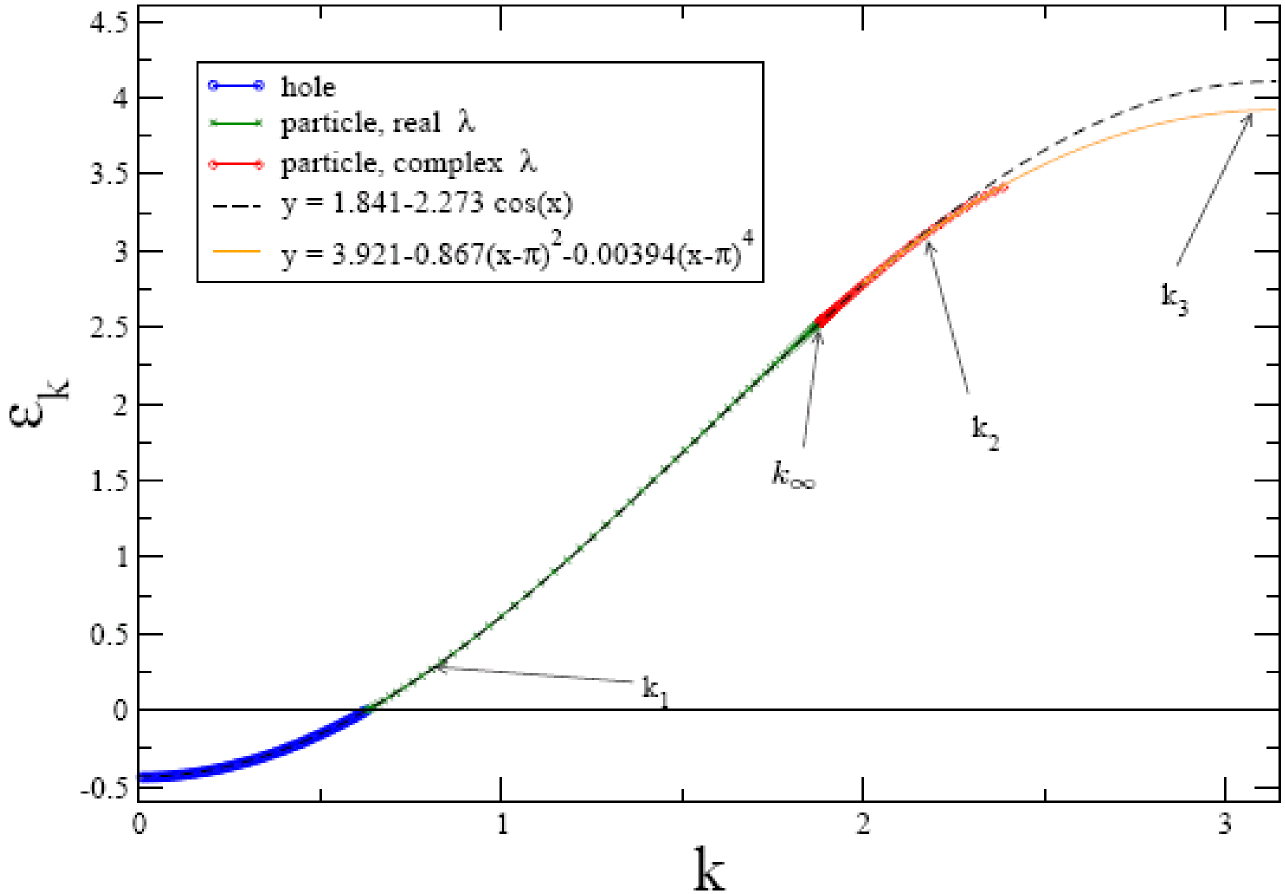
FINITE SIZE SPECTRUM AND BETHE ANSATZ

- Energy and velocity of heavy hole, ε_1, u_1 are determined from Bethe ansatz: $\varepsilon(k)$ is energy to add one hole
- i.e. we remove a single root from ground state (a topological excitation) of momentum k
- $u=d\varepsilon/dk$
- At half-filling (zero field) $\varepsilon(k)=-v \cos k$

$$v = \frac{\pi\sqrt{1-\Delta^2}}{2 \cdot \arccos\Delta}$$

- Away from half-filling $\varepsilon(k)$ appears to be modified in a non-trivial trivial way by the interactions

n=.2 ($\langle S^z \rangle$=-.3), Δ=1/2



- To get $\gamma_{L/R}$, coupling constants between heavy hole and bosonized excitations near Fermi surface, we compare 1/N terms in finite size spectrum
- Without the heavy hole, a low energy excitation with an excess charge, ΔN and D particles transported from left to right Fermi point has excitation energy:

$$\Delta E = \frac{2\pi v}{N}\left[\frac{(\Delta N)^2}{4K} + KD^2 + n_+ + n_-\right]$$

where $n_\pm$ are non-negative integers – the standard Gaussian model result

- The change in ΔN and D under the unitary transformation which eliminates the interaction with the deep hole gives the spectrum with the deep hole present:

$$\Delta N \approx \sqrt{\frac{K}{2\pi}} \int_0^N dx(\partial_x \phi_L - \partial_x \phi_R) \to \Delta N - \frac{\gamma_R + \gamma_L}{2\pi}$$

$$D \approx -\frac{1}{2}\sqrt{\frac{1}{2\pi K}} \int_0^N dx(\partial_x \phi_L + \partial_x \phi_R) \to D - \frac{\gamma_R - \gamma_L}{4\pi K}$$

$$\Delta E = \frac{2\pi v}{N}\left[\frac{1}{4K}\left(\Delta N - \frac{\gamma_R + \gamma_L}{2\pi}\right)^2 + K\left(D - \frac{\gamma_R - \gamma_L}{4\pi K}\right)^2 + n_+ + n_-\right]$$

- The corresponding states, for arbitrary ΔN, D, in the presence of the deep hole, can be constructed from the Bethe ansatz

From Euler-MacLaurin expansion of density of rapidities in presence of the deep hole, we obtain $\Delta E(\Delta N, D)$ in the above form, thus determining $\gamma_{L/R}$

For h=0 we predict, for any q:

$$S(q,\omega \sim \omega_L) \propto \frac{\theta[\omega - v\sin q]}{[\omega - v\sin q]^{1-K}}$$

•Step function at Δ=1 evolves into square root singularity at Δ=1 (Heisenberg model) in agreement with Mueller ansatz and exact 2-spinon result (except for log corrections which are missed in this approach)

At $q \rightarrow 2k_F$, (for $h \neq 0$) we obtain the exponent:

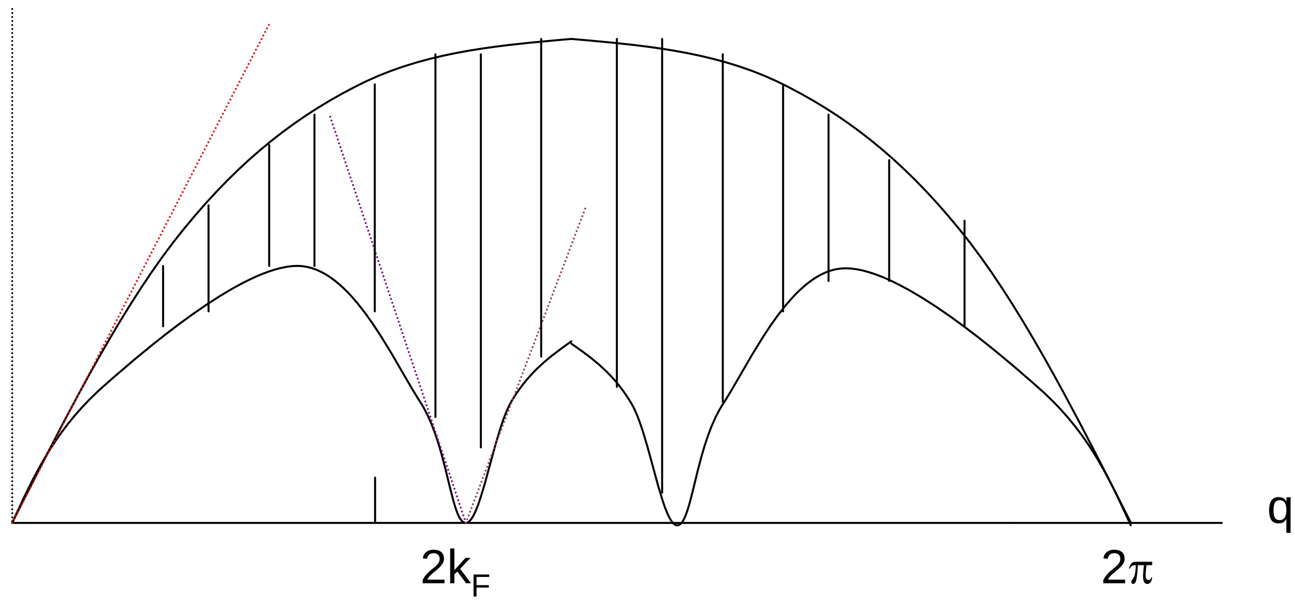
$$1-(\nu_+ + \nu_-) \rightarrow 2\sqrt{K}(1-\sqrt{K})$$

This is different than the well-known Tomonaga-Luttinger liquid result

$$S(q,\omega) \propto \frac{\theta(\omega - v|q-2k_F|)}{[\omega - v(q-2k_F)]^{1-K}[\omega + v(q-2k_F)]^{1-K}}$$

The TLL exponent, 1-K is replaced by $2\sqrt{K}(1-\sqrt{K}) > 1-K$

•The standard TLL theory approximates the dispersion relation as linear, thus giving a higher energy threshold
•We expect that it becomes correct by some sort of crossover at this slightly higher energy scale



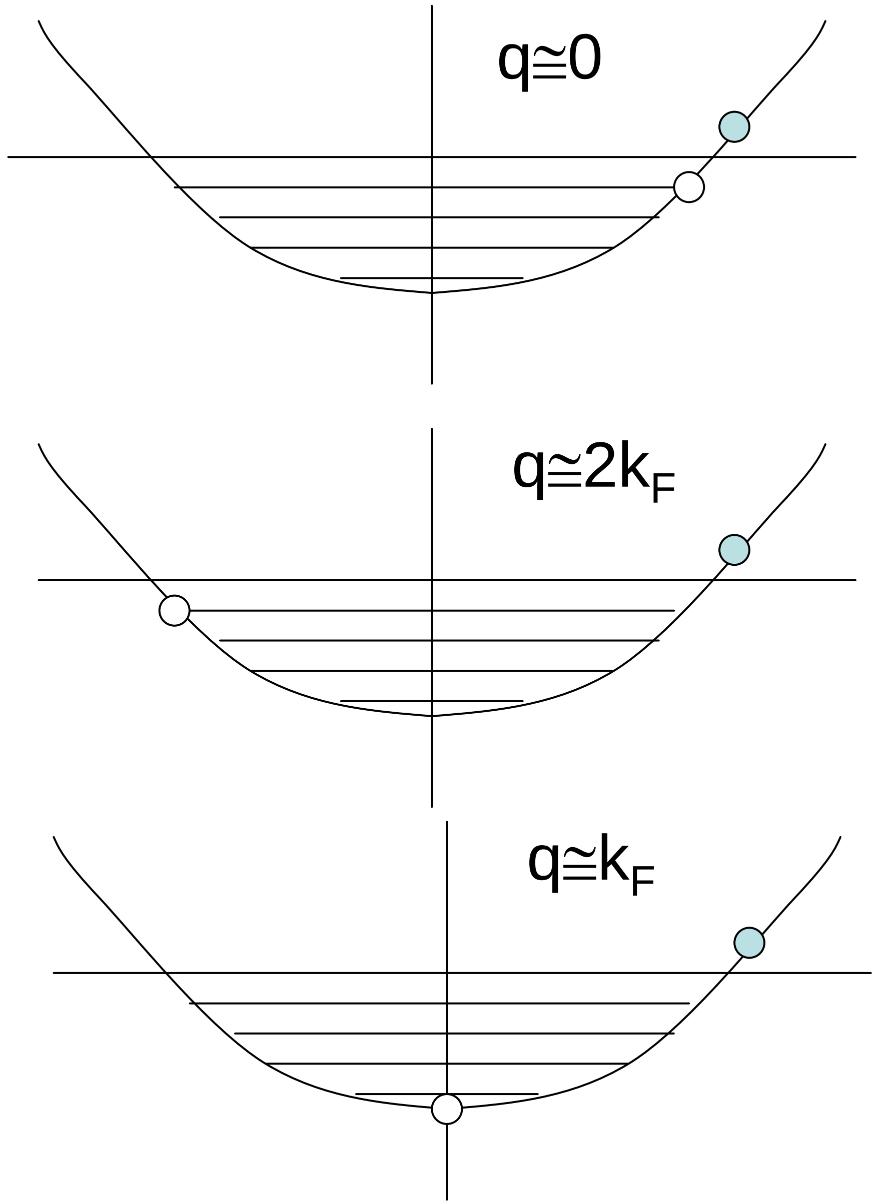
As $q \to 2k_F$, the region of ω where the TLL theory fails shrinks to zero

LONG-TIME BEHAVIOUR OF SELF-CORRELATION FUNCTION

- Our field-theory methods gives directly S(q,t) at long times
- Comparison with DMRG is most direct through G(x,t)
- It is interesting to consider G(x=0,t) at long times

$$G(0,t) = \int_{-\pi}^{\pi} dq S(q,t)$$

At long times, this is dominated by several special values of q:

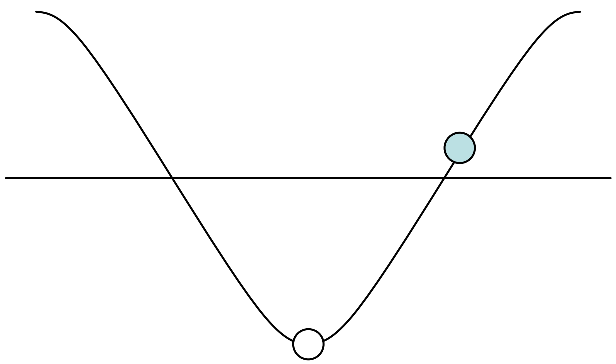


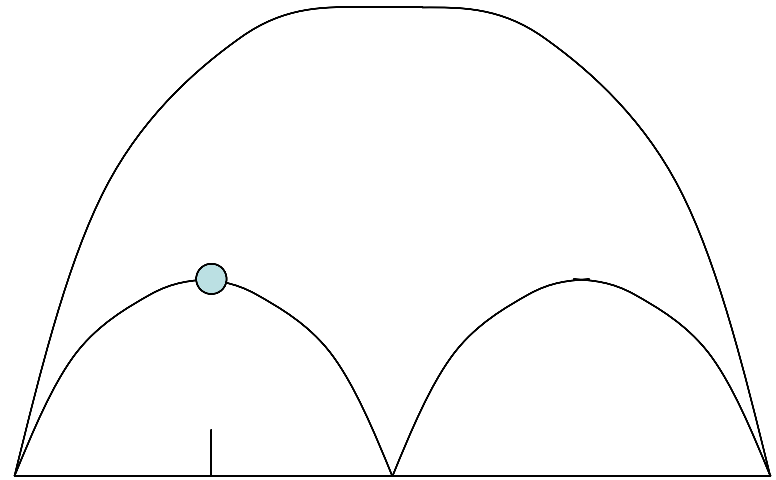
(and others)

- Only q=0 and $\pm 2k_F$ particle-hole pairs are low energy excitations

- Nonetheless other contributions usually dominate at large t!

Consider ½-filling (h=0): hole at k=0, particle at $k=k_F=\pi/2$ dominates





$$\int_{-\pi}^{\pi} dq G(q,t) \rightarrow \int_{-\infty}^{\infty} dq \frac{e^{i\omega_L(q)t}}{t^{\nu_+(q)+\nu_-(q)}}$$

$$\approx \frac{e^{i\omega_L(\pi/2)t}}{t^{\nu_+(\pi/2)+\nu_-(\pi/2)}} \int dq' e^{-i(q'^2/2m)t} \prec \frac{e^{i\nu t}}{t^{\nu_+(\pi/2)+\nu_-(\pi/2)+1/2}}$$

For h=0 we can evaluate $\nu_{\pm}$ explicitly for lower threshold:

$$G(x=0,t) \rightarrow B_1 \frac{e^{-i\nu t}}{t^{K+1/2}} + \frac{B_2}{t^{2K}} + \frac{B_3}{t^2} + \ldots$$

q=π/2 q=π q=0

For 0<Δ<1, ½<K<1, so q=π/2 contribution always dominates

COMPARISON TO DENSITY MATRIX RENORMALIZATION GROUP RESULTS

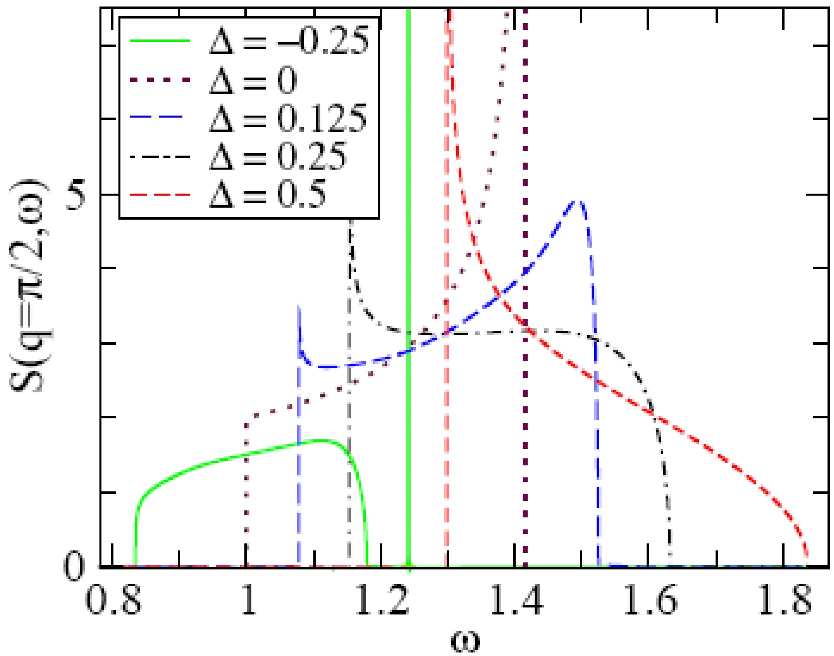
- DMRG is a numerical, iterative, variational approach that gives excellent accuracy for 1D quantum systems at T=0
- Recently generalizations have been found which give real time correlation functions out to moderate times with good accuracy
- Keeping up to 400 lattice sites and 1000 states we can get G(x,t) out to times of 30 – 60 (in units of 1/J=1) with errors of order 10^{-4} -10^{-5}
- We can then Fourier transform in x

•For 10<t<30 we compare DMRG to field theory/Bethe ansatz predictions – checking predicted frequencies and exponents
•Once we are convinced it works we can supplement DMRG for short to intermediate times with asymptotic results out to infinite time – the time-Fourier transform can then be performed without usual rounding of singularities due to finiteness of time interval

Δ	W	v	η	$\frac{1}{2}+K$
0	1	1	1.5	1.5
0.125	1.078	1.078	1.451	1.426
0.25	1.153	1.154	1.366	1.361
0.375	1.226	1.227	1.313	1.303
0.5	1.299	1.299	1.287	1.25
0.75	1.439	1.438	1.102	1.149

h=0, lower edge energy and exponent from G(0,t)
•Similar comparison works well for G_F

Fourier transformed DMRG + field theory data for h=0



CONCLUSIONS

- Luttinger-liquid theory fails to describe some critical features of 1D many body systems
- Limited progress can be made by including

higher dimension operators in bosonized Hamiltonian

- “X-ray edge” methods, combined with Bethe ansatz

predict new critical exponents that seem to agree
with DMRG calculations

- Open questions remain regarding decay of “heavy

hole” and robustness of critical singularities, among
other topics