# Diffusive versus Ballistic Transport in 1 Dimensional Quantum Systems

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# Outline

- Introduction,
- bosonization review
- Mazur bound
- Perturbative calculation
- tDMRG results
- $1/T_1$ in Heisenberg spin chains: $Sr_2CuO_3$
- Conclusions and open questions

# 1. Introduction

- dc conductivities of normal metals are finite at T>0, even in absence of impurities
- Re [σ(ω]) has a finite peak at ω=0 with width given by inelastic scattering rate
- Related behavior predicted in magnetic materials:

$$< S^z_{\vec{q}}(t) S^z_{-\vec{q}}(0) > \to \exp[-\mathrm{D}q^2 t]$$

for a ferromagnet at long times (DeGennes) where D(T) is diffusion constant

- This is normal, diffusive transport

In 1 dimension, spinless tight-binding model of metal is directly related to antiferromagnet by Jordan-Wigner transformation:

$$S_j^z = c_j^+ c_j - 1/2, \;\; S_j^- = (-1)^j \exp\left[ i\pi \sum_{k<j} c_k^+ c_k \right] c_j$$

$$H = \sum_j \left[ -t(c_j^+ c_{j+1} + h.c.) + V\hat{n}_j \hat{n}_{j+1} \right]$$

$$= \sum_j [J(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z) - hS_j^z]$$

$$J = t, \;\; \Delta = V/t, h = \mu$$

Charge current operator of electron model is spin current of spin model:

$$J_l = -it(c_l^+ c_{l+1}^- - h.c.) = -\frac{iJ}{2}(S_l^+ S_{l+1}^- - h.c.)$$

$$J_T \equiv \sum_l J_l$$

Charge conductivity (spin conductivity) given by Kubo formula:

$$\sigma(\omega) = \frac{i}{\omega L}\left[< E_{kin} > + < J_T J_T >_{ret} (\omega)\right]$$

- In principle, conductivity may have a non-zero Drude weight, $D$(T), defined by

$\mathrm{Re}\,\sigma(\omega)=2\pi D(T)\delta(\omega)+\sigma_{reg}(\omega)$

- This is known as *ballistic transport* and isn't generally expected, except at T=0
- However, it was shown that $D$ (T)>0 *, for all T* for above Hamiltonian, for a range of parameters (Mazur, Suzuki, Zotos et al., Prosen)
- Proof uses integrability of model – existence of an operator, *Q that* commutes with H and has a non-zero overlap with current operator: $\langle J_T Q\rangle\neq 0$

For h≠0, we may use $Q=J_{E,T}$, energy current operator, defined by:

$$\partial_t H_j = -i[H_j, H] = -(J_{E,j} - J_{E,j-1}),$$

$$J_{E,j} = J^2[S^y_{j-1}S^z_j S^x_{j+1} - S^x_{j-1}S^z_j S^y_{j+1} + \Delta(S^x_{j-1}S^y_j S^z_{j+1} - S^z_{j-1}S^y_j S^x_{j+1})$$
$$+\Delta(S^z_{j-1}S^x_j S^y_{j+1} - S^y_{j-1}S^x_j S^z_{j+1})]$$
$$= J^2(\vec{S}_{j-1} \times \vec{S}_j)\cdot \vec{S}_{j+1} \text{ (for } \Delta = 1)$$

$$J_{E,T} = \sum_j J_{E,j}$$

- This is just the first non-trivial member of an infinite family of *local* conserved quantities, obeying $[J^{(n)},H]=0$, in this integrable model obtained from transfer matrix

- Many (but not all) experts believe that this is a special feature of integrable model and that diffusive behavior: D(T)=0 for T>0,
would be recovered as soon as integrability is broken, for example by adding 2nd neighbor hopping or interactions
- At half filling (h=0) $\langle J_E J \rangle = 0$
- Tomaz Prosen found a matrix product quasi-local conserved operator which gives a non-zero Mazur bound at h=0, for $\Delta<1$, vanishing at $\Delta \rightarrow 1$

# 2. Perturbative Calculation

- At low T we may use field theory methods: bosonization, renormalization group
$c_j \approx \exp[ik_F j]\psi_R(j) + \exp[-ik_F j]\psi_L(j)$
where $\psi_{L/R}$ vary slowly
- We then bosonize resulting Dirac theory
- $J\Delta\psi_L^+\psi_L\psi_R^+\psi_R$ term leaves boson model free, with shifted Luttinger parameter, K
- $J\Delta(\psi_L^+\psi_L^+\psi_R\psi_R \exp(4ik_F j) + h.c.)$ Umklapp term is non-oscillating at $k_F=\pi/2$ (half-filling, h=0) and gives sine-Gordon interaction in bosonized model

$$H = \frac{1}{2}\left[\Pi^2 + v\left(\frac{d\phi}{dx}\right)^2\right] + \lambda\cos\left(\sqrt{8\pi K}\phi\right)$$

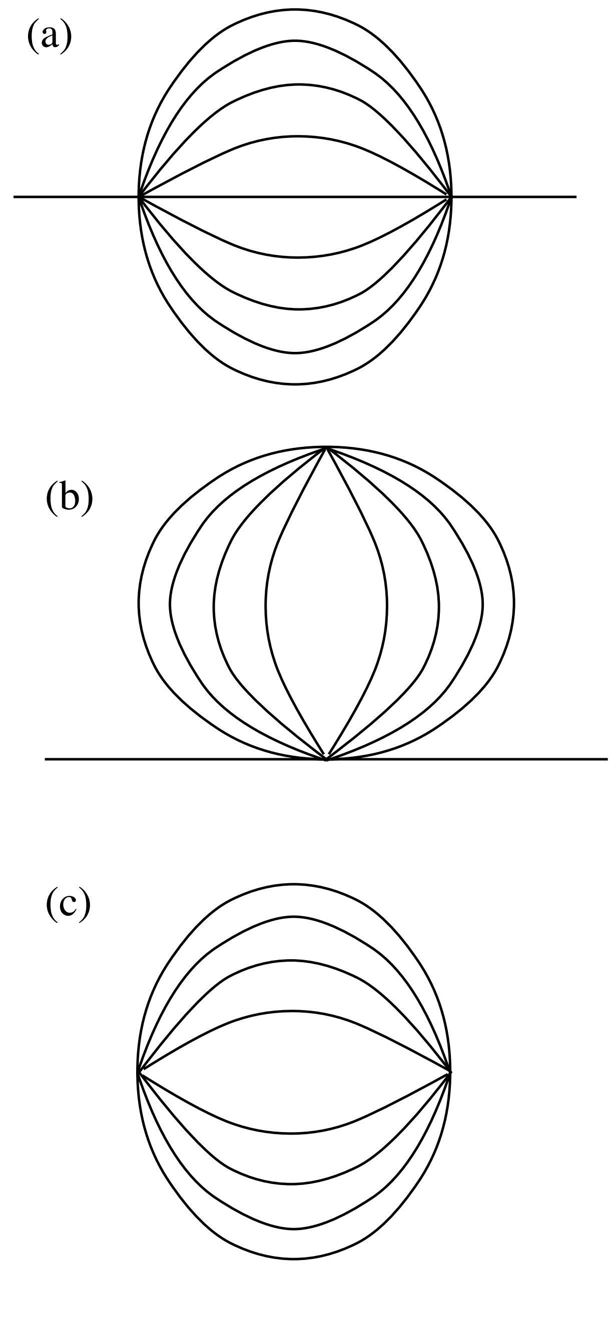
- Umklapp term (sine-Gordon interaction) is irrelevant for $\Delta \leq 1$ ($K \geq 1$) where model is gapless
- For $\Delta \leq 1$ we can ignore it at T=0 and we should be able to treat it perturbatively at $T \ll J$, even when bare $\lambda/v \sim \Delta$ is not small
- charge (spin) current in bosonized model is:

$J(x) = -\mathrm{v}\sqrt{K/2\pi}\,\Pi(x)$ giving conductivity: $\sigma(q,\omega)=(K/2\pi)i\omega\langle\phi\phi\rangle_{ret}(q,\omega)$. Ignoring Umklapp and other irrelevant operators,

$\sigma(0,\omega)=\sigma(\omega)=(iKv/2\pi)/(\omega+i\varepsilon)$, independent of T

$\mathrm{Re}\,[\sigma(\omega)]=(Kv/2)\delta(\omega)$- purely a Drude peak

Feynman diagrams for self energy to second order in sine-Gordon interaction



- Including Umklapp, and other interactions, gives a self energy $\Pi(q,\omega)$ to $\phi$-field and thus:
- $\sigma(\omega)=(iKv\omega/2\pi)/[\omega^2-\Pi(0,\omega)]$.
- Umklapp term gives an imaginary term in $\Pi(\omega)$ in second order: $\Pi(\omega)=-2i\Gamma(T)\omega$ with $\Gamma(T)\sim\lambda^2T^{4K-3}$ (at zero field)
- M. Oshikawa and I calculated $\Pi(q,\omega)$ in 1997 for Electron Spin Resonance theory
- $\Gamma(T)$ is the inelastic scattering rate
- It gives conductivity a Lorentzian form (with D=0): $\sigma(\omega)\approx(iKv/2\pi)/[\omega+2i\Gamma(T)]$

- Using input from Bethe ansatz (Lukyanov & Zamalodchikov) exact coupling constant $\lambda$ of Umklapp term can be determined and hence exact coefficient, $c(K)$, in $\Gamma=c(K)T^{4K-3}$
- For Heisenberg model, $\Delta=1$, Umklapp becomes part of a marginal interaction ~g and: $2\Gamma(T)=\pi g(T)^2 T$, with $g(T)\sim 1/\ln(T_0/T)$, $T_0=2.87\ J$

- While this all looks quite standard and convincing this cannot be completely correct!

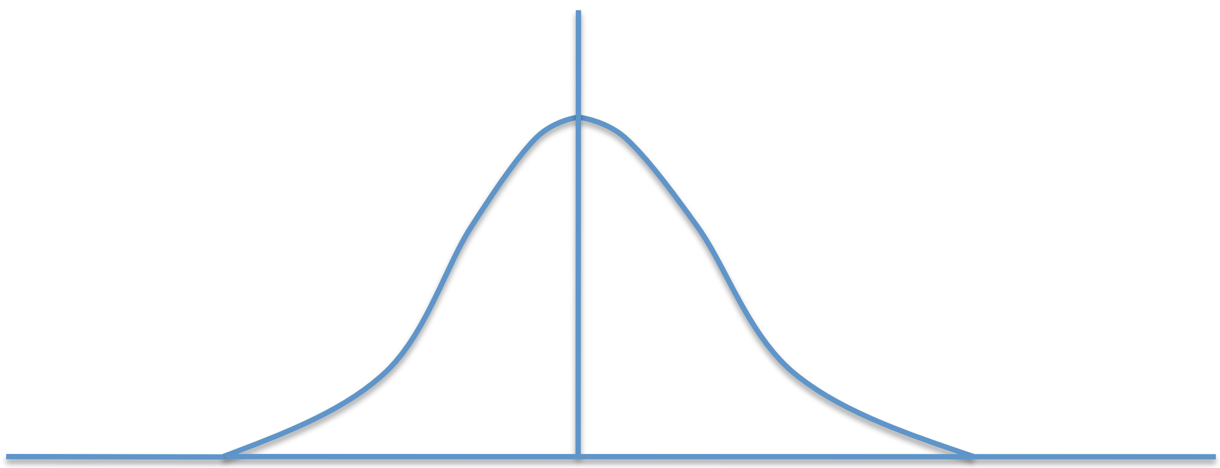
Prosen's Mazur bound gives a non-zero Drude weight, at $h=0$ for $\Delta<1$

- Should we throw out this calculation? What's wrong with it? We believe it is correct, as far as it goes (eg. gives good agreement with ESR data and also NMR data – see below).
- However, it may be necessary to include higher order terms in perturbation theory at low $\omega \sim \Gamma(T)y$
- $\Pi(\omega) \approx -2i\Gamma\omega/[1+y2i\Gamma/\omega]$ where y controls Drude weight: $y = \langle JQ\rangle^2/[\langle J\rangle^2\langle Q\rangle^2 - \langle JQ\rangle^2]$, Q conserved

  $D = Kvy/[2\pi(1+y)]$
- We have obtained corresponding result for $\sigma(\omega)$ from "memory matrix" approach – method for including effects of integrability (Rosch & Andrei)

This ansatz gives a conductivity:

$$\mathrm{Re}\,\sigma(\omega) = \frac{vK}{2\pi}\left[\frac{\pi y}{1+y}\delta(\omega) + \frac{2\Gamma}{\omega^2 + 4\Gamma^2(1+y)^2}\right]$$



A linear superposition of a Lorentzian and Delta-function: diffusive + ballistic transport

- Width of Lorentian is approximately $\Gamma(T)$ as before
- $y(h,T)$ controls fraction of spectral weight in Drude peak
- Can this form of $\Pi(\omega)$ be obtained by summing some infinite family of Feynman diagrams that mix J with conserved quantity, with y controlling mixing?

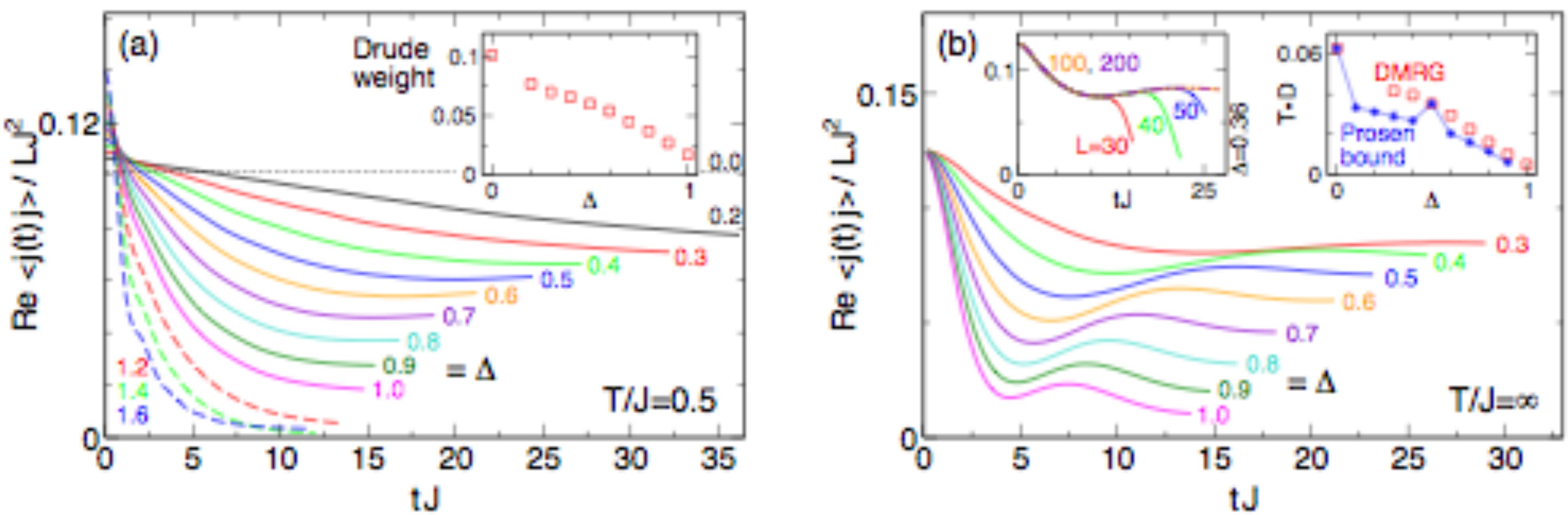
$\Pi \sim -ic\lambda^2\omega/[1-iyc\lambda^2/\omega]$

- "Conserving approximation" needed.

# 3. Numerical Results

- While Monte Carlo (Alvarez & Gross, Grossjohan & Brenig) and exact diagonalization (Heidrich-Meisner et al.) have been applied to calculate the Drude weight, real-time finite temperature Density Matrix Renormalization Group (tDMRG) techniques are most effective.
- $C(t,T)=\langle J_T(t)J_T\rangle(T)$ is calculated out to fairly large t. $\lim_{t\to\infty} C(t,T)/(2LT)=D(T)$.
- The main numerical limitation is the maximum value of time, t, that can be reached.

# DMRG Results on Drude Weight



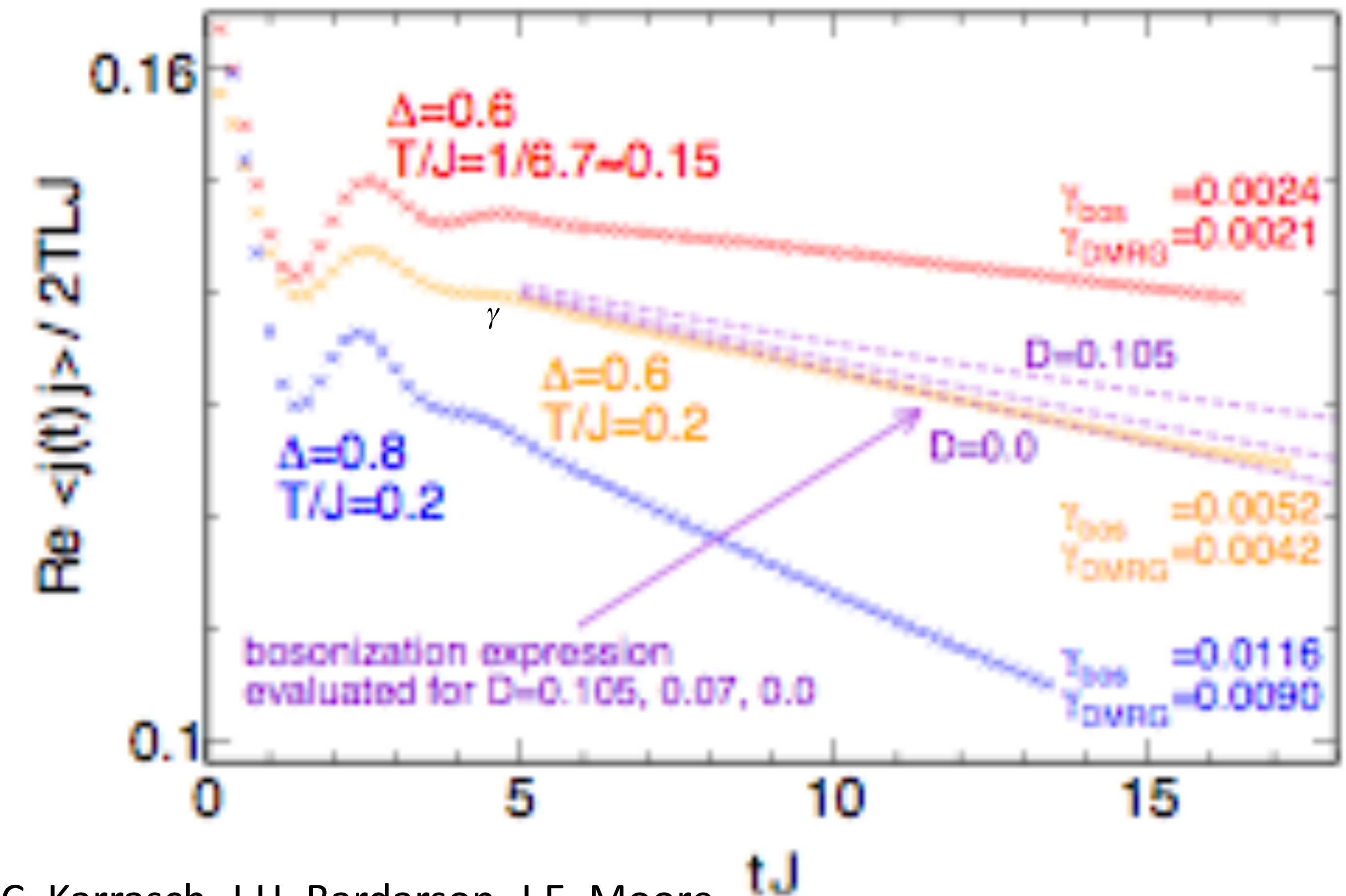

C. Karrasch, J.H. Bardarson, J.E. Moore, Phys. Rev. Lett. 108, 227206 (2012)

At low $T \ll J$, where field theory may work, we expect exponential decay if $D=y=0$: $C(t) \sim \exp[-2\Gamma t]$. Our ansatz, for non-zero y gives a constant plus exponentially decaying term, at $\Gamma, 1/t \ll T \ll J$:

$$C(t) = \frac{vKT}{2\pi(1+y)}\left[y + e^{-2\Gamma(1+y)t}\right]$$

At intermediate times, $\Gamma \ll 1/t \ll T \ll J$, this is linear and independent of y: $C(t) \approx (vKT/2\pi)(1-2\Gamma t)$

DMRG data at low T can be well- fit by this formula allowing Γ to be extracted and D to be estimated. Γ from DMRG agrees quite well with bosonization.

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Phys. Rev. Lett. 108, 227206 (2012)

# 4. $1/T_1$ in Heisenberg Spin Chains

A static magnetic field h, is applied to the nuclei in a magnet, then a small transverse oscillating field is applied, to induce nuclear spin transitions. Adsorption intensity versus frequency exhibits a peak broadened around resonance frequency due to coupling of nuclear spin to atomic spins. Width, $1/T_1$, is $2^{nd}$ order in hyperfine coupling. For static field in z-direction:

$$\frac{1}{T_1} = \frac{1}{2}\int \frac{dq}{2\pi}\left|A(q)\right|^2 < S^+S^- > (q,\omega_N,h,T)$$

- $A(q)$ is hyperfine coupling form factor
- $\omega_N$ is nuclear magnetic resonance frequency: $\omega_N=(\mu_N/\mu_B)h \approx 0$
- for Heisenberg model in a weak field $h<<T$, we may approximate this finite field transverse Green's function by a zero field longitudinal one $<S^+S^->(\omega=0,h)\approx 2<S^zS^z>(\omega=h,0)$

- This follows since $H=H_0-hS^z_T$ where $[H_0,S^z_T]=0$
So, $S^+_l(t)=\exp[-iht]\exp[iH_0t]S^+_l\exp[-iH_0t]$
- $-hS^z_T$ also appears in Boltzmann weights in calculating Green's function, but is negligible for $h<<T<<J$
- Normally $1/T_1$ is dominated by $q\approx\pi$ region where $\langle S^zS^z\rangle(q,h)$ diverges
- However, if $A(q)$ vanishes at $q=\pi$, $q\approx 0$ region can dominate and $1/T_1$ is related to diffusive behavior of $\langle\phi\phi\rangle(q,\omega)$. In this case:

$$\frac{1}{T_1} = \int \frac{dq}{2\pi} A(q)^2 \frac{2\,\mathrm{Im}\,\chi_{ret}(q,\omega = h)}{1 - e^{-h/T}}$$

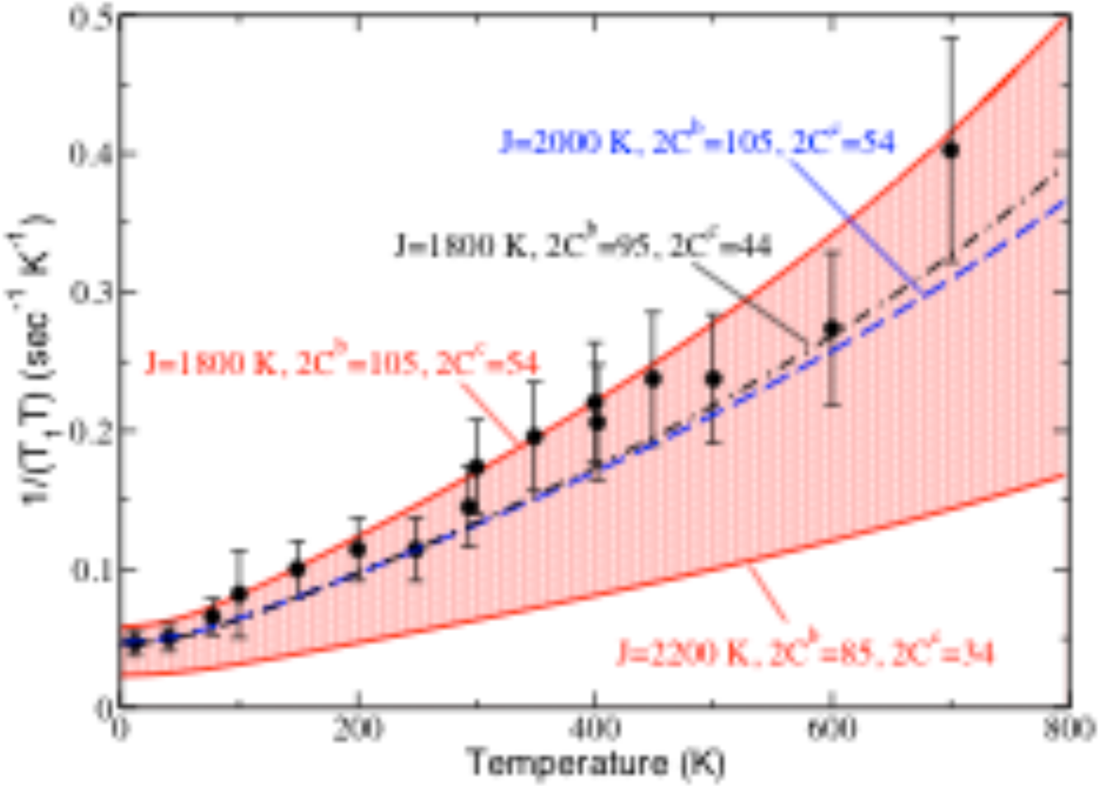
$$\approx 2\frac{T}{h} A(0)^2 2\Gamma h \int_{-\infty}^{\infty} \frac{dq}{2\pi} \frac{vq^2/(2\pi)}{(vq)^4 + (2\Gamma h)^2} \quad (\text{for } h << T)$$

$$= A^2 \frac{2}{\pi^3 J^2} T \sqrt{\frac{\Gamma(T)}{h}}$$

$$\frac{1}{T_1 T} \approx A^2 \frac{2}{\pi^3 J^2} \sqrt{\frac{\pi T}{2h \ln^2(J/T)}}$$

(Here we are ignoring ballistic term in <ϕϕ> which appears to be zero or very small for $h \approx 0$ and $\Delta = 1$.)

- These conditions are all met for NMR on in-chain O-ions in $Sr_2CuO_3$
- This material contains Cu-O-Cu-O-Cu chains, similar to some cuprate superconductors
- $J \approx 2000$ K and Néel order only occurs at very suppressed temperature, $T_N \approx 10$ K
- Location of in-chain O-ions in between a pair of magnetic Cu ions cancels hyperfine coupling at $q=\pi$, $A(q)=A\cos(q/2)$
- J and A are known from susceptibility and Knight shift measurements so we can make a zero parameter fit to theory

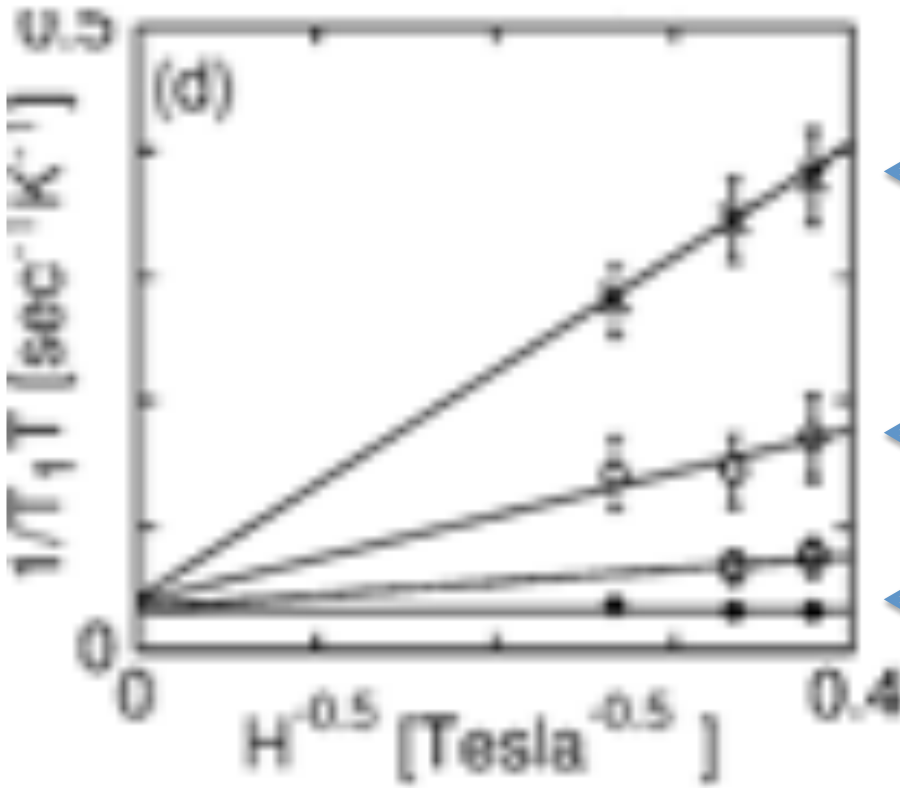



$Sr_2CuO_3$

•K. Thurber et al., PRL 87, 247202 (2001) (Takashi Imai's group)

•Allowing for 20% uncertainties in J and A, agreement is quite good (although largest T may be a bit high for field theory approximation)

Thurber et al fitted the field-dependence of their data to $h^{-1/2}$. (Only 3 data points at 2 temperatures!)




295 K

77 K

(different O-site or material, ignore)

# 5. Conclusions and Open Question

- Lowest order field theory calculation predicts a Lorentzian form for conductivity at low T
- For Heisenberg model at zero field this result agrees quite well with tDMRG data and $1/T_1$ experimental data on $Sr_2CuO_3$
- There is an additional Drude peak at $\Delta<1$ which appears to coexist with Lorentzian
- Can coexistence formula be derived from summing Feynman diagrams?
- Additional experimental/numerical data for $1/T_1$?

J. Sirker, R.G. Pereira and I.A., PRB 83, 035115 (2011)