Adiabatic-antiadiabatic crossover in a spin-Peierls chain

E. Orignac
École Normale Supérieure/CNRS UMR 7549,
France
R. Citro
Università di Salerno/Unità INFM di Salerno,
Italy
T. Giamarchi
Université de Genève, DPMC, Switzerland

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Spin-Peierls dimerization

$$H = \sum_n \Big[(1+g(u_{n+1}-u_n))(J(S^x_n S^x_{n+1} + S^y_n S^y_{n+1}) + J_z S^z_n S^z_{n+1}) + \frac{k_e}{2}(u_{n+1}-u_n)^2 + \frac{p_n^2}{2M}\Big]$$

$g = 0$: XXZ spin 1/2 chain $\Rightarrow$ gapless for $\Delta \leq 1$.

$g \neq 0$:

(a) $M \to \infty$: Adiabatic limit.

$\Rightarrow \langle u_{n+1} - u_n \rangle = (-)^n \delta$.

$\Rightarrow$ spin gap $\Delta \sim J(g\delta)^{2/3}$ $(J_z = J)$

$\Rightarrow$ energy gain $E_0(\delta) \sim -J(g\delta)^{4/3}$ (up to log. corrections)

Elastic energy cost $K\delta^2/2$.

Balance:

$\Rightarrow \Delta \sim \frac{(Jg)^2}{k_e}$

Spontaneous spin-Peierls dimerization (Cross, Fisher, 1979).

spin Peierls dimerization II

(b) $M \to 0$: Antiadiabatic limit.

Phonon frequency: $\omega_0 \sim \sqrt{k_e/M} \to \infty$

$\Rightarrow$ integrate out phonons.

2nd order P.T. (Kuboki, Fukuyama, 1987)

$$H = \sum_n \left[\left(J + \frac{(Jg)^2}{8k_e} \right) \mathbf{S}_n \cdot \mathbf{S}_{n+1} + \frac{(Jg)^2}{16k_e} \mathbf{S}_n \cdot \mathbf{S}_{n+2} \right]$$

Frustrated spin chain.

$\Rightarrow$ Opening of the gap only if the frustration is large enough ($J_2/J_1 > 0.24$).

Crossover between these 2 regimes ??

Bosonized representation

$$
\begin{aligned}
S &= \int dx \int_0^\beta \frac{d\tau}{2\pi K}\left[u(\partial_x\phi)^2 + \frac{1}{u}(\partial_\tau\phi)^2\right] \\
&\quad -\frac{(Jg)^2}{2\pi^2\alpha k_e}\int dx \int_0^\beta d\tau \int_0^\beta d\tau' \cos 2\phi(x,\tau) \\
&\quad \times\mathcal{D}_{\omega_0,\beta}(\tau-\tau')\cos 2\phi(x,\tau'),
\end{aligned}
$$

Phonons have been integrated out.

$$
K^* = \frac{1}{2-\frac{2}{\pi}\arccos\left(\frac{J_z}{J}\right)}
$$

$$
u^* = \frac{\pi}{2}\frac{\sqrt{J^2-J_z^2}}{\arccos\left(\frac{J_z}{J}\right)}\alpha
$$

$$
\mathcal{D}_{\omega_0,\beta}(\tau) = \text{phonon propagator}
$$

$$
\omega_0 \sim (k_e/M)^{1/2}
$$

$$
\mathcal{D}_{\omega_0,\beta}(\tau-\tau') = \langle q(\tau)q(\tau')\rangle =
$$

$$
\frac{\omega_0}{2}\left[e^{-\omega_0|\tau-\tau'|} + \frac{2\cosh(\omega_0(\tau-\tau'))}{e^{\beta\omega_0}-1}\right].
$$

The two limits

- the adiabatic limit:

$\omega_0 \to 0 \Rightarrow \mathcal{D}_{\omega_0,\beta}(\tau) \sim 1/\beta \Rightarrow$ mean-field limit (Cross and Fisher).

$\Delta \sim J(Jg^2/k_e)^{1/(2-2K)}$

- the antiadiabatic limit:

$\omega_0 \to \infty \Rightarrow \mathcal{D}_{\omega_0,\beta}(\tau) \sim \delta(\tau)$

$\Rightarrow \int \mathcal{D} \cos 2\phi \cos 2\phi \sim \cos 4\phi$

$K > 1/2$: irrelevant $\Rightarrow$ no gap for $g < g_c$

$K = 1/2$: marginal ($\leftrightarrow$ XXX chain)

$K < 1/2$: relevant

Crossover can be studied within SCHA in the limit $K < 1/2$.

Self-consistent harmonic approximation

Trial action:

$$S_0 = \int dx \int_0^\beta \frac{d\tau}{2\pi K}\left[u(\partial_x\phi)^2 + \frac{1}{u}(\partial_\tau\phi)^2 + \frac{\Delta^2}{u}\phi^2\right],$$

where Δ= Gap.

Variational principle:

$$F_{\text{var.}} = F_0 + \langle S - S_0\rangle_0 \geq F,$$

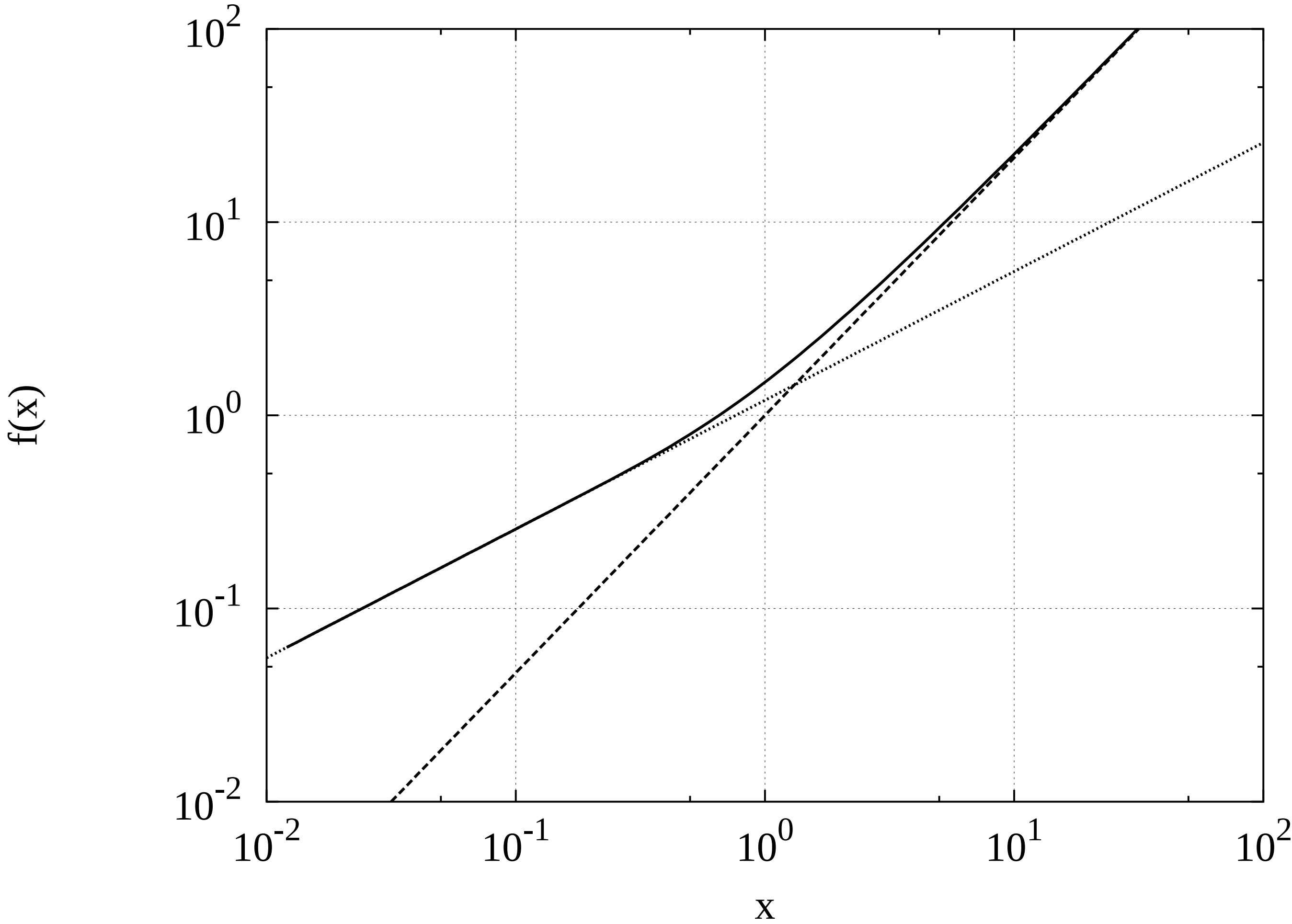
Minimization w.r.t. Δ

$$f\left(\frac{\Delta}{\omega_0}\right) = \frac{4K(Jg)^2}{\pi u k_e \alpha}\left(\frac{u}{\omega_0\alpha}\right)^{2-2K}\left(\frac{e^{\gamma_E}}{2}\right)^{2K},$$

where:

$$f(x) = \frac{x^{2-2K}}{e^{-2\frac{e^{-\gamma_E}}{x}} + \left(x\frac{e^{\gamma_E}}{2}\right)^{2K}\gamma\left(1+2K, 2\frac{e^{-\gamma_E}}{x}\right)}$$

Crossover for $K < 1/2$



• $x \ll 1 \Rightarrow f(x) \sim x^{2-4K}$: Antiadiabatic limit

$$\Delta \sim \frac{u}{\alpha} \left[\frac{(Jg)^2}{k_e u \alpha} \left(\frac{u}{\alpha \omega_0} \right)^{2K} \right]^{\frac{1}{2-4K}}$$

• $x \gg 1 \Rightarrow f(x) \sim x^{2-2K}$: Adiabatic limit

(Cross-Fisher, 1979)

$$\Delta_{CF} \sim \frac{u}{\alpha} \left[\frac{(Jg)^2}{k_e u \alpha} \right]^{\frac{1}{2-2K}}$$

Crossover for $\Delta_{CF} \sim \omega_0$.

Renormalization group approach

$$
\begin{aligned}
S &= \int dx \int_0^\beta \frac{d\tau}{2\pi K}\left[u(\partial_x\phi)^2 + \frac{1}{u}(\partial_\tau\phi)^2\right] \\
&- \frac{\alpha}{2k_e}\left(\frac{Jg}{\pi\alpha}\right)^2 \int dx \int_0^\beta d\tau \int_0^\beta d\tau' \cos 2\phi(x,\tau) \\
&\times \mathcal{D}_{\omega_0,\beta}(\tau-\tau')\cos 2\phi(x,\tau') \\
&- \frac{2g_\perp}{(2\pi a)^2}\int dx \int_0^\beta d\tau \cos 4\phi(x,\tau).
\end{aligned}
$$

$\cos(4\phi) \rightarrow$ generated by the RG flow.

$$
\begin{aligned}
&\frac{d}{dl}\left(\frac{1}{K}\right) = \left(\frac{g_\perp}{\pi u}\right)^2 + \frac{(Jg)^2}{\pi u k_e \alpha}\frac{\alpha}{u}\mathcal{D}_{\omega_0(l)}(\frac{\alpha}{u}), \\
&\frac{d}{dl}\left(\frac{g_\perp}{\pi u}\right) = (2-4K)\frac{g_\perp}{\pi u} + \frac{(Jg)^2}{\pi u k_e \alpha}\frac{\alpha}{u}\mathcal{D}_{\omega_0(l)}(\frac{\alpha}{u}), \\
&\frac{d}{dl}\left(\frac{(Jg)^2}{\pi u k_e \alpha}\right) = \left(2(1-K) + \frac{g_\perp}{\pi u}\right)\frac{(Jg)^2}{\pi u k_e \alpha}, \\
&\frac{d\omega_0}{dl} = \omega_0.
\end{aligned}
$$

$K < 1/2$

Two step RG (Bourbonnais, Caron 1984):

• Step 1: Renormalize up to the scale $\omega_0 e^{l_0} \sim u/\alpha$.

$\rightarrow g_\perp(l_0) \sim \frac{(Jg)^2}{\pi u k_e \alpha}\left(\frac{u}{\alpha\omega_0}\right)^{2K}$

Unless a gap is formed at the scale $\Delta_{CF} \sim \frac{u}{\alpha}\left(\frac{(Jg)^2}{\pi u k_e \alpha}\right)^{1/(2-2K)} \ll \omega_0$

• Step 2: Gap $\Delta \sim g_\perp(l_0)^{1/(2-4K)}$

Equivalent to SCHA.

At $K \simeq 1/2$, marginal operator $\cos 4\phi \Rightarrow$ breakdown of SCHA.

The case of the XXX chain

$$K = \frac{1}{2}\left(1 - \frac{g_\perp}{2\pi u}\right).$$

$y = \frac{g_\perp}{\pi u} < 0, G = \frac{(Jg)^2}{\pi u k_e \alpha}$.

$$\frac{dy}{dl} = y^2 + G(l)\frac{\omega_0 \alpha}{2u} e^l e^{-\frac{\omega_0 \alpha}{u} e^l}$$
$$\frac{dG}{dl} = \left(1 + \frac{3}{2}y\right) G$$

Applying the 2-step RG:

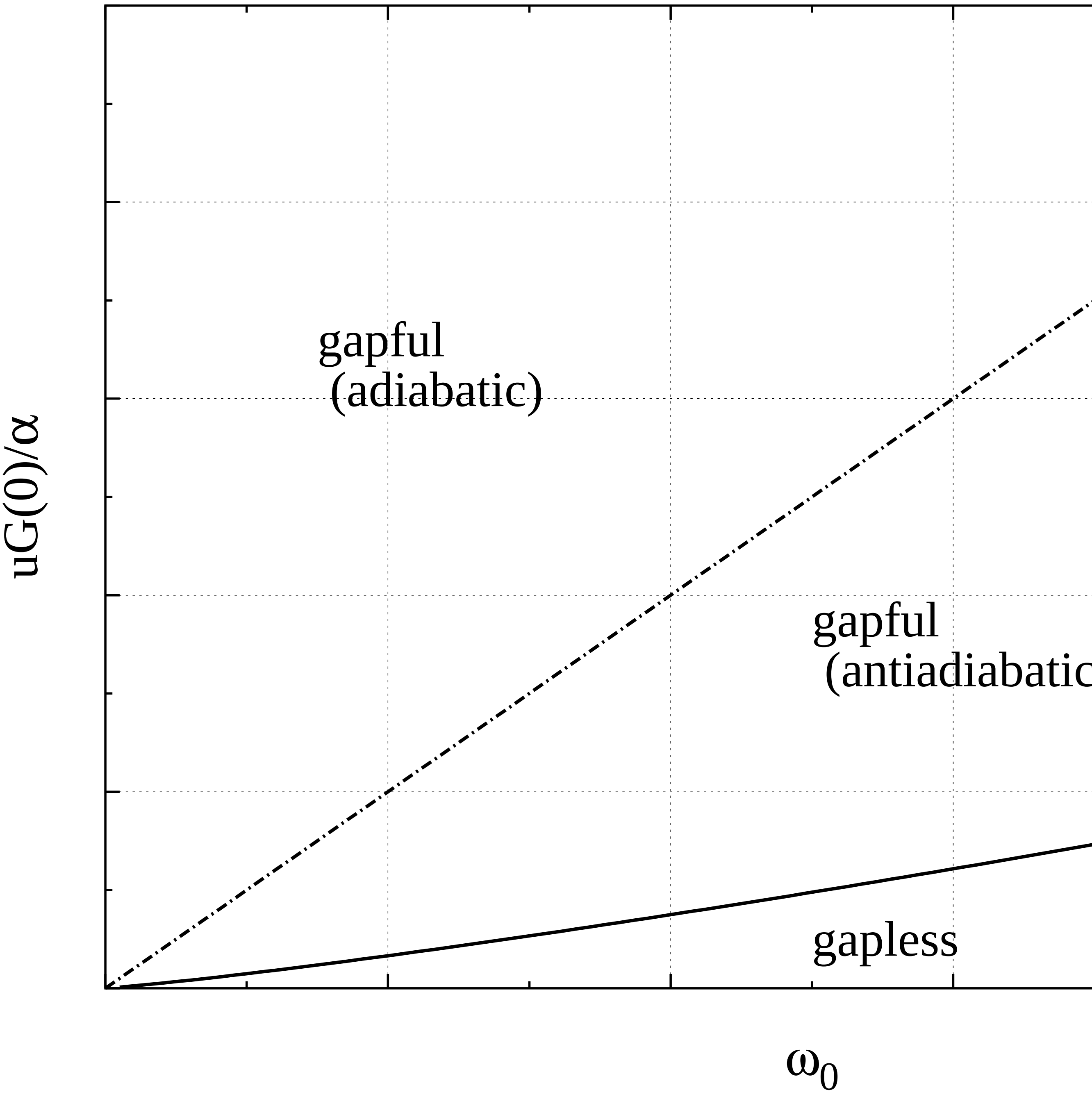
Gap exists only if:

$$\frac{uG(0)}{2\omega_0 \alpha} > \frac{|y(0)|}{1 + |y(0)| \ln\left(\frac{ue^{1-\gamma}}{\alpha\omega_0}\right)}.$$

For $\omega_0 \gg \Delta_{CF} \sim \frac{u}{\alpha} G(0)$:

$$\Delta \sim \omega_0 \exp\left[\frac{-1}{\frac{uG(0)}{2\omega_0\alpha} + \frac{y(0)}{1 - y(0)\ln\frac{ue^{1-\gamma}}{\omega_0 \alpha}}}\right]$$

Otherwise: $\Delta \sim \Delta_{CF}$


gapful
(adiabatic)
gapful
(antiadiabatic
gapless
uG(0)/α
ω0

Conclusions

1. Crossover adiabatic/antiadiabatic regime in the XXX chain for $\Delta_{ad.} \sim \omega_0$.
2. Adiabatic regime, $\Delta \sim g^2/k_e \gg \omega_0$
3. Antiadiabatic regime
$\Delta \sim \omega_0 e^{-Cte.k_e/(g^2-g_c^2(\omega_0))} \ll \omega_0$
4. At higher frequency or for $g < g_c(\omega_0)$, KT phase transition gapful-gapless.