Impact of partially bosonized collective fluctuations on electronic degrees of freedom

V.Harkov*, M. Vandelli, A. I. Lichtenstein, E. A. Stepanov/ *arXiv: 1908.00536 (2019)*
European X-Ray Free-Electron Laser Facility, 22869 Schenefeld, Germany
I. Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany
* viktor.harkov@xfel.eu

European XFEL

Mean-field approach

$$\mathcal{S} = -\sum_{\mathbf{k},\nu} c^*_{\mathbf{k}\nu}\mathcal{G}^{-1}_{\mathbf{k}\nu}c_{\mathbf{k}\nu} + U\sum_{\mathbf{q},\omega} n_{\mathbf{q}\omega\uparrow}n_{-\mathbf{q},-\omega\downarrow} + \frac{1}{2}\sum_{\mathbf{q},\omega,\varsigma} V^{\varsigma}_{\mathbf{q}}\rho^{\varsigma}_{\mathbf{q}\omega}\rho^{\varsigma}_{-\mathbf{q},-\omega}$$

$$\mathcal{G}_{\mathbf{k}\nu} = [i\nu + \mu - \varepsilon_{\mathbf{k}}]^{-1}; \quad \rho^{\varsigma} = n^{\varsigma} - \langle n^{\varsigma}\rangle; \quad \varsigma = \{c, s\}$$

Bosonization (*H-S transformation*)

$$Un_{\uparrow}n_{\downarrow} = \frac{1}{2}U^{c}nn + \frac{1}{2}U^{s}\vec{m}\,\vec{m} \rightarrow -\frac{1}{2}\phi^{\varsigma}\left[U^{\varsigma}\right]^{-1}\phi^{\varsigma} + \phi^{\varsigma}c^*_{\sigma}\vec{\sigma}^{\varsigma}_{\sigma\sigma'}c_{\sigma'}$$

$$U^{s} = \frac{1}{3}(U^{c} - U); \quad \boxed{U^{c} - \text{arb.}}$$

- *All diagrams — exact solution*
- *Approximate solution — Fierz ambiguity problem*

GW approximation

Standard formulation: $U^{c} = U; \; U^{s} = 0$

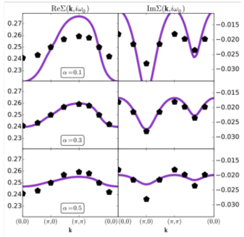
$$W^{c}_{\mathbf{q}\omega} = \frac{U + V_{\mathbf{q}}}{1 - \Pi_{\mathbf{q}\omega}(U + V_{\mathbf{q}})}$$

motivation: charge Vq

"Spin GW": $U^{c} = 0; \; U^{z} = -U$

$$W^{s}_{\mathbf{q}\omega} = \frac{-U}{1 + \Pi_{\mathbf{q}\omega}U}$$

motivation: $\Pi U < 0$



T. Ayral et al. / *PRL* **119**, 166401 (2017)

Partially bosonized dual theory

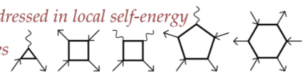
Dual Boson approach

$$\mathcal{S} = -\sum_{\mathbf{k},\nu} c^*_{\mathbf{k}\nu}\mathcal{G}^{-1}_{\mathbf{k}\nu}c_{\mathbf{k}\nu} + U\sum_{\mathbf{q},\omega} n_{\mathbf{q}\omega\uparrow}n_{-\mathbf{q},-\omega\downarrow} + \frac{1}{2}\sum_{\mathbf{q},\omega,\varsigma} V^{\varsigma}_{\mathbf{q}}\rho^{\varsigma}_{\mathbf{q}\omega}\rho^{\varsigma}_{-\mathbf{q},-\omega}$$

$$\downarrow$$

$$\tilde{\mathcal{S}} = -\sum_{\mathbf{k},\nu,\sigma} f^*_{\mathbf{k}\nu\sigma}\tilde{\mathcal{G}}^{-1}_{\mathbf{k}\nu\sigma}f_{\mathbf{k}\nu\sigma} - \frac{1}{2}\sum_{\mathbf{q},\omega,\varsigma}\varphi^{\varsigma}_{\mathbf{q}\omega}\tilde{\mathcal{W}}^{\varsigma\,-1}_{\mathbf{q}\omega}\varphi^{\varsigma}_{-\mathbf{q},-\omega} + \tilde{\mathcal{F}}[f,\varphi^{\varsigma}]$$

- Green's functions - *nonlocal* and *dressed in local self-energy*
- Bare interaction = *full local vertices*
- **No Fierz ambiguity**



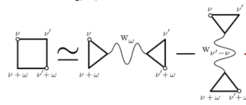
Back from the dual space $\varphi^{\varsigma} \rightarrow b^{\varsigma}$

$$\tilde{\mathcal{S}} = -\sum_{\mathbf{k},\nu,\sigma} f^*_{\mathbf{k}\nu\sigma}\tilde{\mathcal{G}}^{-1}_{\mathbf{k}\nu\sigma}f_{\mathbf{k}\nu\sigma} - \frac{1}{2}\sum_{\mathbf{q},\omega,\varsigma}\varphi^{\varsigma}_{\mathbf{q}\omega}\tilde{\mathcal{W}}^{\varsigma\,-1}_{\mathbf{q}\omega}\varphi^{\varsigma}_{-\mathbf{q},-\omega} + \varphi^{\varsigma}\triangleleft^{f}_{f^*} + {}^{f^*}_{f}\square^{f}_{f^*}$$

H-S transformation

$$\mathcal{S}_{f\text{-}b} = -\sum_{\mathbf{k},\nu,\sigma} f^*_{\mathbf{k}\nu\sigma}\tilde{\mathcal{G}}^{-1}_{\mathbf{k}\nu\sigma}f_{\mathbf{k}\nu\sigma} - \frac{1}{2}\sum_{\mathbf{q},\omega,\varsigma} b^{\varsigma}_{\mathbf{q}\omega}W^{\varsigma\,-1}_{\mathbf{q}\omega}b^{\varsigma}_{-\mathbf{q},-\omega} + b^{\varsigma}\triangleleft^{f}_{f^*}$$

Approximation:



w=?

Approximation for the vertex

$$\mathcal{S}^{(i)}_{\text{imp}} = -\sum_{\nu,\sigma} c^*_{\nu\sigma}[i\nu + \mu - \Delta_{\nu}]c_{\nu\sigma} + U\sum_{\omega} n_{\omega\uparrow}n_{-\omega\downarrow} + \frac{1}{2}\sum_{\omega,\varsigma}\Lambda^{\varsigma}_{\omega}\,\rho^{\varsigma}_{\omega}\,\rho^{\varsigma}_{-\omega}$$

$$\mathcal{U}^{\varsigma}_{\omega} = U^{\varsigma} + \Lambda^{\varsigma}_{\omega}$$

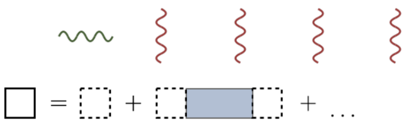
$$\frac{1}{2}\sum_{\omega,\varsigma}\mathcal{U}^{\varsigma}_{\omega}\rho^{\varsigma}_{\omega}\,\rho^{\varsigma}_{-\omega}$$

antisymmetrization

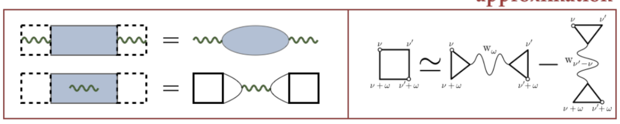
$$\frac{1}{8}\sum_{\nu,\nu',\omega}\sum_{\varsigma,\sigma(')}\Gamma^{0\,\varsigma}_{\nu\nu'\omega}c^*_{\nu\sigma}\sigma^{\varsigma}_{\sigma\sigma'}c_{\nu+\omega,\sigma'}c^*_{\nu'+\omega,\sigma''}\sigma^{\varsigma}_{\sigma''\sigma'''}c_{\nu',\sigma'''}$$

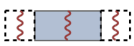
$$\Gamma^{0\,c}_{\nu\nu'\omega} = \boxed{2\mathcal{U}^{c}_{\omega}} - \mathcal{U}^{c}_{\nu'-\nu} - \mathcal{U}^{x}_{\nu'-\nu} - \mathcal{U}^{y}_{\nu'-\nu} - \mathcal{U}^{z}_{\nu'-\nu} = \boxed{U} + \ldots$$

$$\Gamma^{0\,z}_{\nu\nu'\omega} = \boxed{2\mathcal{U}^{z}_{\omega}} - \mathcal{U}^{z}_{\nu'-\nu} + \mathcal{U}^{x}_{\nu'-\nu} + \mathcal{U}^{y}_{\nu'-\nu} - \mathcal{U}^{c}_{\nu'-\nu} = \boxed{-U} + \ldots$$

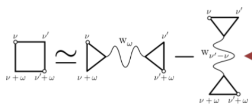


approximation



 **<— not included in the approximation**

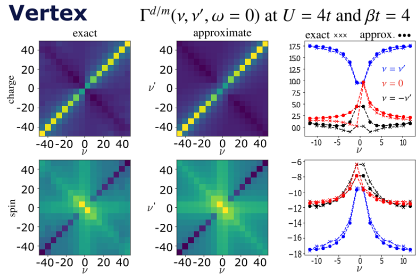
$$U^{c} = U/2$$
$$U^{s} = -U/2 \quad \nleftrightarrow \quad U^{s} = \frac{1}{3}(U^{c} - U)$$



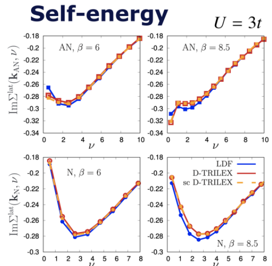
$$\boxed{w_{\omega} = W^{\text{imp}}_{\omega} - U^{\varsigma}/2}$$

D-TRILEX

Vertex $\Gamma^{d/m}(\nu, \nu', \omega = 0)$ at $U = 4t$ and $\beta t = 4$



Self-energy $U = 3t$

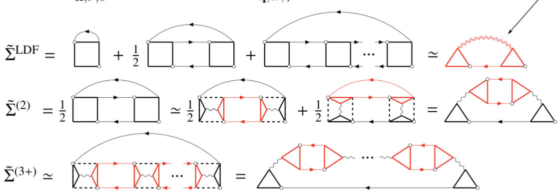


D-TRILEX Self-energy

$$\boxed{W^{\varsigma}_{\mathbf{q}\omega} = W^{\text{EDMFT}}_{\mathbf{q}\omega} - U^{\varsigma}/2}$$

$$\mathcal{S}_{f\text{-}b} = -\sum_{\mathbf{k},\nu,\sigma} f^*_{\mathbf{k}\nu\sigma}\tilde{\mathcal{G}}^{-1}_{\mathbf{k}\nu\sigma}f_{\mathbf{k}\nu\sigma} - \frac{1}{2}\sum_{\mathbf{q},\omega,\varsigma} b^{\varsigma}_{\mathbf{q}\omega}W^{\varsigma\,-1}_{\mathbf{q}\omega}b^{\varsigma}_{-\mathbf{q},-\omega} + b^{\varsigma}\triangleleft^{f}_{f^*}$$

$$\tilde{W}^{\varsigma}_{\mathbf{q}\omega} = \frac{(U^{\varsigma} + V^{\varsigma}_{\mathbf{q}})}{1 - \Pi^{\varsigma}_{\mathbf{q}\omega}(U^{\varsigma} + V^{\varsigma}_{\mathbf{q}})}$$



Self-energy

$$\Sigma^{\text{latt}}_{\mathbf{k}\nu\sigma} = \Sigma^{\text{imp}}_{\nu} + \Sigma'_{\mathbf{k}\nu\sigma},$$

$\Sigma'_{\mathbf{k}\nu\sigma} =$

Polarization operator

$$\Pi^{\varsigma\,\text{latt}}_{\mathbf{q}\omega} = \Pi^{\varsigma\,\text{imp}}_{\omega} + \Pi'_{\mathbf{q}\omega},$$

$\Pi'_{\mathbf{q}\omega} =$