Various Fermi liquid phases on the Kondo-Heisenberg model at quarter filling

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Introduction

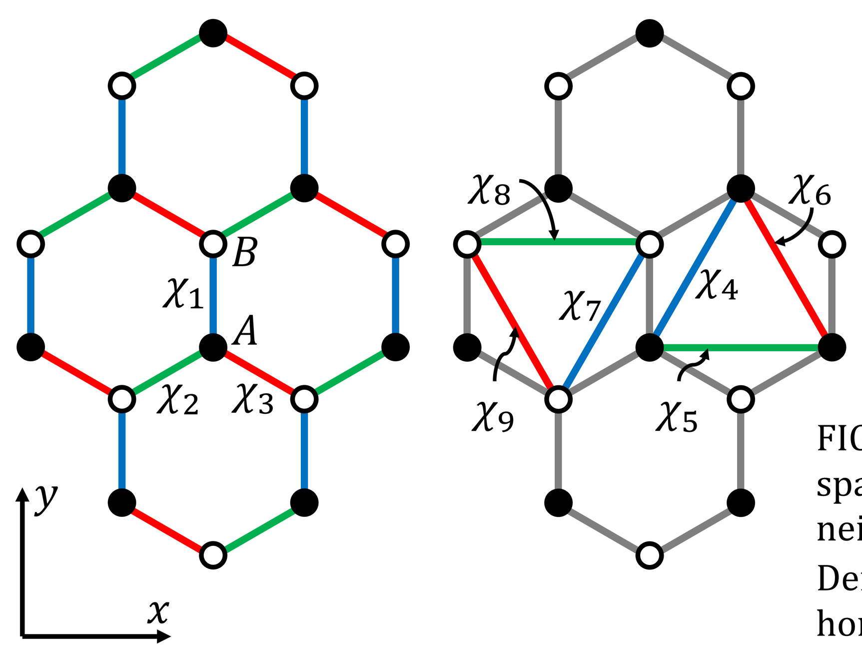
1. Motivation

- Paramagnetic heavy fermion compound of Kondo-lattice system was reported (e.g. $CeRh_2Si_2$, CePdAl, etc.).
- What is the effect of interplaying between magnetic frustration and Kondo physics?

2. Kondo – Heisenberg model

$$\hat{H}_{\mathrm{KH}} = -\sum_{\langle i,j\rangle,\alpha}\left(\hat{c}^{\dagger}_{i,\alpha}\hat{c}_{j,\alpha} + h.c.\right) + \frac{J_K}{2}\sum_{i,\alpha,\beta}\hat{c}^{\dagger}_{i,\alpha}\vec{\sigma}_{\alpha\beta}\hat{c}_{i,\beta}\cdot\hat{\vec{S}}_i + J_1\sum_{\langle i,j\rangle}\hat{\vec{S}}_i\cdot\hat{\vec{S}}_j + J_2\sum_{\langle\langle i,j\rangle\rangle}\hat{\vec{S}}_i\cdot\hat{\vec{S}}_j$$

- $\hat{c}^{\dagger}_{i,\alpha}$: Itinerant electron creation operator at site i with spin α
- $\hat{\vec{S}}_i$: Localized spin operator at site i with spin magnitude $S = 1/2$
- $\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$: Pauli matrices



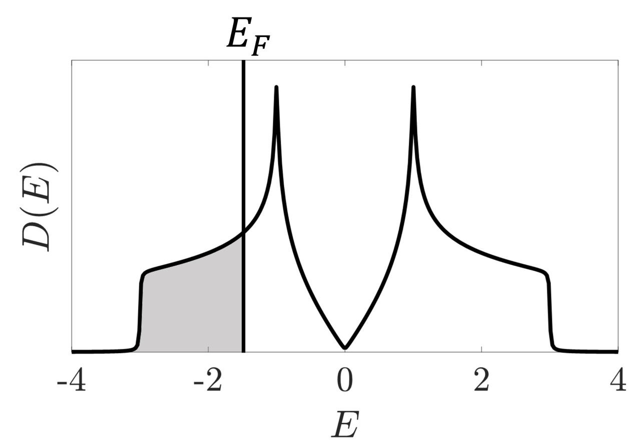


FIG. 1. Honeycomb lattice structure in the real space and definition of nearest/next nearest neighboring bond order parameters χ_{ij}. Density of state for tight binding model on the honeycomb lattice is presented.

Methods

1. Spinon representation & Mean-field theory

1-1) Spinon representation

$$\hat{\vec{S}}_i = \tfrac{1}{2}\Sigma_{\alpha,\beta}\hat{f}^{\dagger}_{i,\alpha}\vec{\sigma}_{\alpha\beta}\hat{f}_{i,\beta} \text{ with } \hat{H}_{\mathrm{KH}} \to \hat{H}_{\mathrm{KH}} + \Sigma_{i,\alpha}\lambda_i(\hat{f}^{\dagger}_{i,\alpha}\hat{f}_{i,\alpha} - 1)$$

- $\hat{f}^{\dagger}_{i,\alpha}$: Charge neutral fermion creation operator at site i with spin α
- λ_i : Lagrange multiplier

1-2) Mean-field theory & Self-consistency equation

$$\hat{H}^{\mathrm{MFT}}_{\mathrm{KH}} = \left(-\sum_{\langle i,j\rangle,\alpha}\hat{c}^{\dagger}_{i,\alpha}\hat{c}_{j,\alpha} - \frac{J_K}{2}\sum_i b_i\hat{c}^{\dagger}_{i,\alpha}\hat{f}_{i,\alpha} - \frac{J_1}{2}\sum_{\langle i,j\rangle}\chi_{ij}\hat{f}^{\dagger}_{j,\alpha}\hat{f}_{i,\alpha} - \frac{J_2}{2}\sum_{\langle\langle i,j\rangle\rangle}\chi_{ij}\hat{f}^{\dagger}_{j,\alpha}\hat{f}_{i,\alpha} + h.c.\right) + \sum_{i,\alpha}\lambda_i(\hat{f}^{\dagger}_{i,\alpha}\hat{f}_{i,\alpha} - 1) - \mu\sum_{i,\alpha}\hat{c}^{\dagger}_{i,\alpha}\hat{c}_{i,\alpha}$$ (up to constant energy shift)

- $\chi_{ij} = \Sigma_\alpha\langle\hat{f}^{\dagger}_{i,\alpha}\hat{f}_{j,\alpha}\rangle$: Spinon hopping order parameter
- $b_i = \Sigma_\alpha\langle\hat{f}^{\dagger}_{i,\alpha}\hat{c}_{i,\alpha}\rangle$: Kondo singlet order parameter

2. Electric conductivity & Thermal conductivity

2-1) Electric conductivity

$$\sigma_{\mu\nu}(T) = \int dE[-\partial_E f(E,T)]\xi_{\mu\nu}(E)$$

Kubo formula

$$\xi^c_{\mu\nu}(E) = \frac{1}{\pi N_b N_c}\sum_{b=1}^{N_b}\sum_{\boldsymbol{k}\in\mathrm{BZ}}^{N_c}\left(\left|c^{(b)}_{\boldsymbol{k},A}\right|^2 + \left|c^{(b)}_{\boldsymbol{k},B}\right|^2\right)v^{(b)}_\mu(\boldsymbol{k})v^{(b)}_\nu(\boldsymbol{k})\left[\mathrm{Im}G^{(b)}(\boldsymbol{k},E)\right]^2$$

- $f(E,T)$: Fermi-Dirac Distribution
- $c_{\boldsymbol{k},\alpha}$: Itinerant electron coefficient of eigenvector at momentum $\boldsymbol{k}$

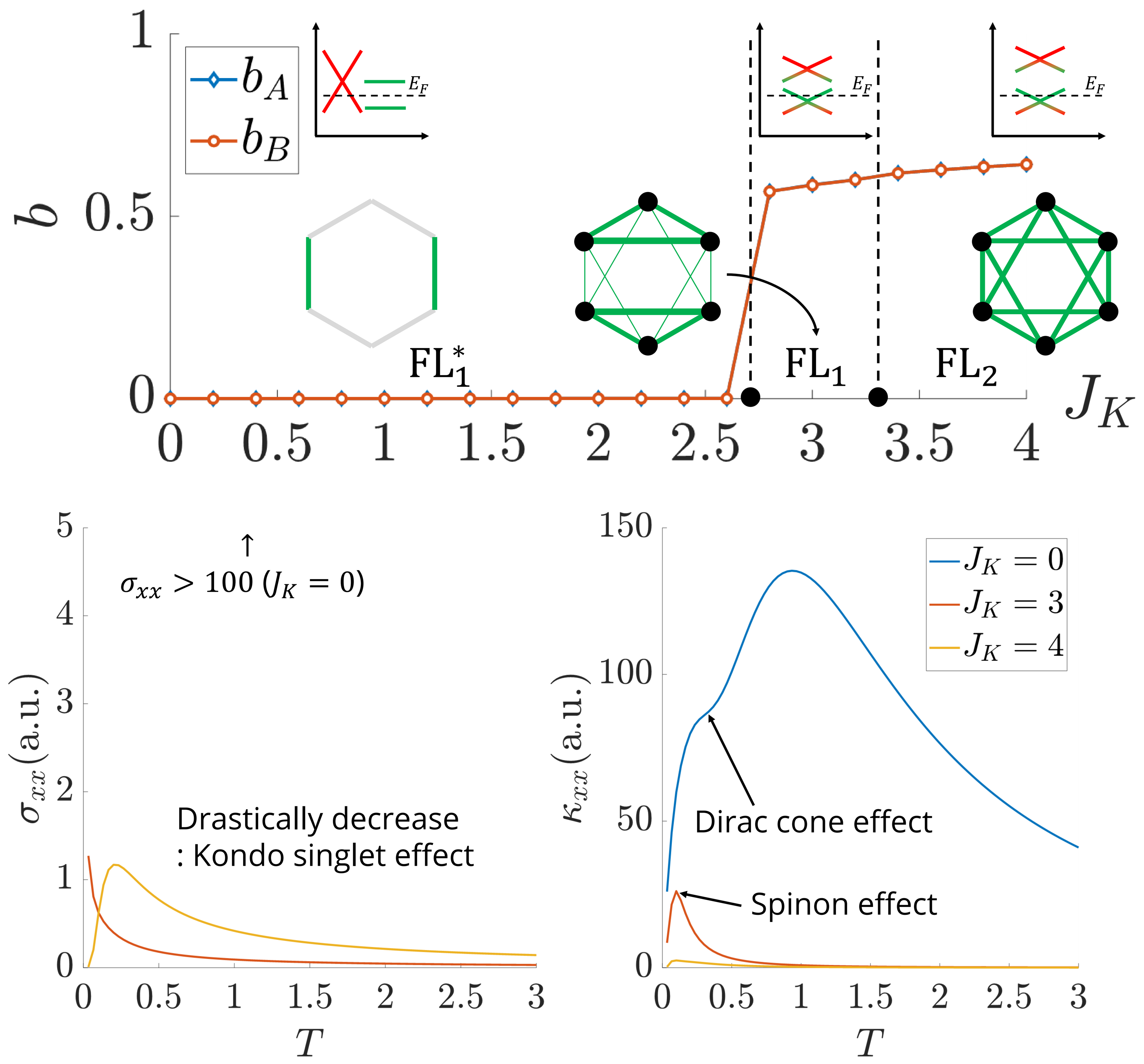
2-2) Thermal conductivity

$$\kappa_{\mu\nu}(T) = \frac{1}{T^2}\left\{L^2_{\mu\nu}(T) - \frac{\left[L^1_{\mu\nu}(T)\right]^2}{L^0_{\mu\nu}(T)}\right\}^2 \qquad \zeta_{\mu\nu}(E,T) = T\xi(E)$$

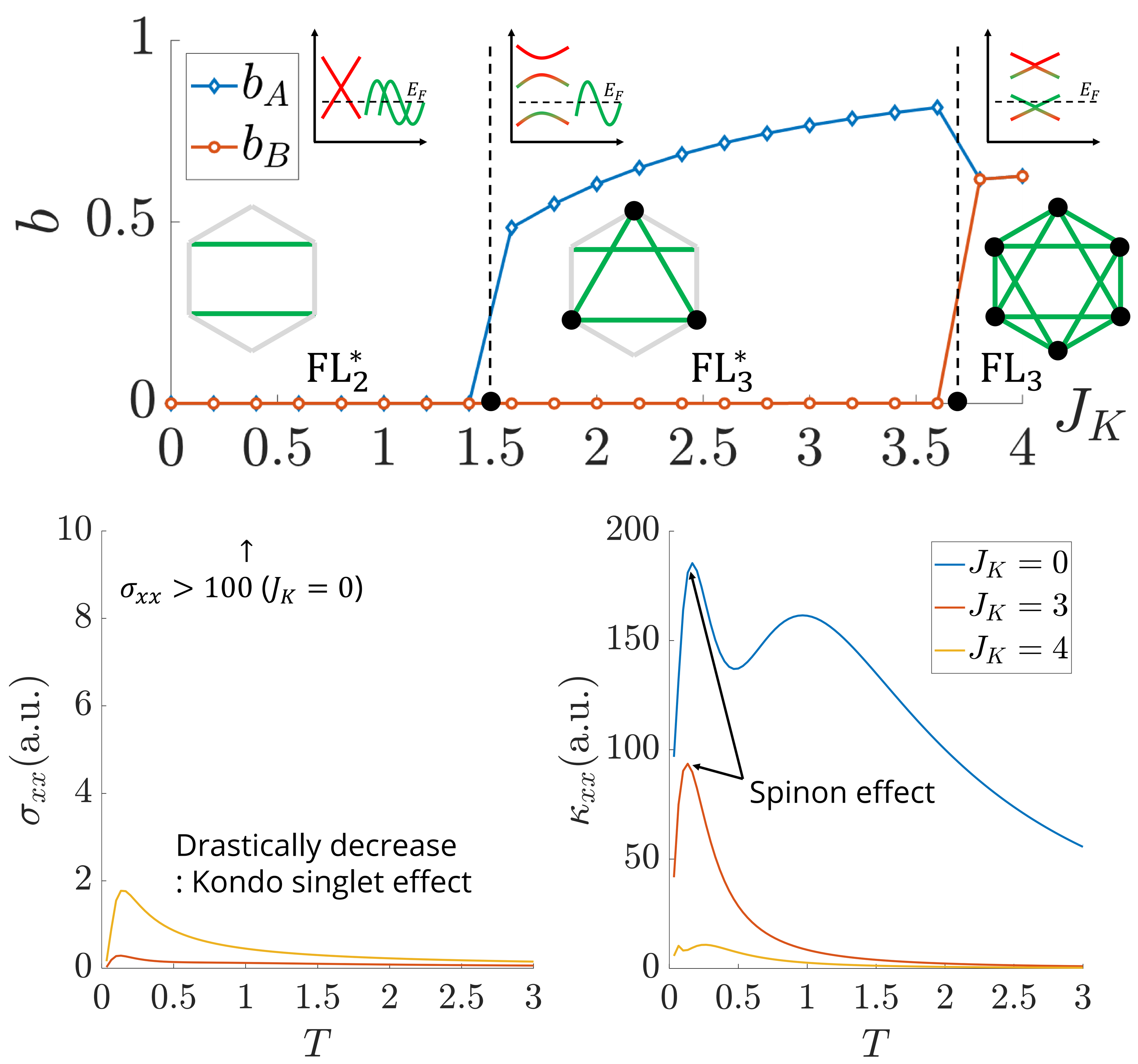
- $L^n_{\mu\nu}(T) = \int dE[-\partial_E f(E,T)]\zeta_{\mu\nu}(E,T)E^n$: Transport coefficients

Results

1. $J_1 = 1$ & $J_2 = 0.5$ case



2. $J_1 = 0.5$ & $J_2 = 1$ case



Conclusions

- Interplay of Magnetic frustration and Kondo coupling leads to partial Kondo screening with phase transition between FL and FL*.
- For intermediate Kondo coupling $J_K^* < J_K < J_K^{**}$, partial Kondo screening results in charge gap near T_K and emergent low energy spinon excitation below T_K.
- (Partial) Kondo screening drastically changes electrical and thermal transport properties due to charge gap and large spinon contribution.