Disorder correction to the Neel temperature of ruthenium-doped $BaFe_2As_2$: Theoretical analysis

S.V. Kokanova[1, 3] and A.V. Rozhkov[1, 2, 3]

[1]*Moscow Institute of Physics and Technology (State University), Institutsky lane 9, Dolgoprudny, Moscow region, 141700 Russia*

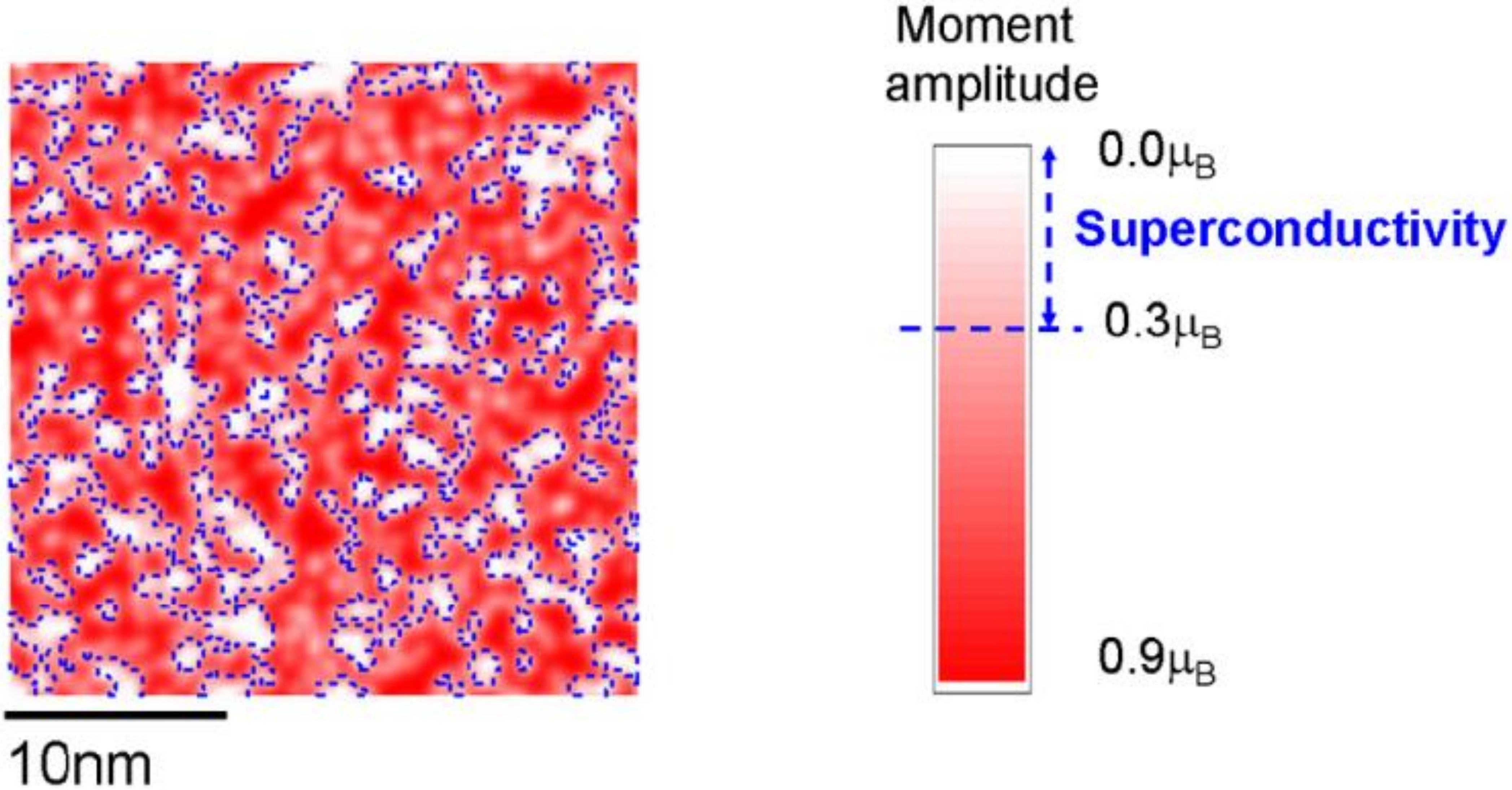
[2]*Institute for Theoretical and Applied Electrodynamics, Moscow, 125412 Russia*

[3]*Skolkovo Institute of Science and Technology, Skolkovo Innovation Center 3, Moscow 143026, Russia*

Plan

- Motivation
- Model
- Calculation
- Analysis of experimental data
- Summary

$BaFe_{2(1-x)}Ru_{2x}As_2$



Y. Laplace, J. Bobroff, V. Brouet, G. Collin, F. RullierAlbenque, D. Colson, and A. Forget, Phys. Rev. B **86**, 020510 (2012).

Model

The Landau free energy functional:

$$F[S(\mathbf{r})] = \int \left\{ C_{\|}\left[(\nabla_x S)^2 + (\nabla_y S)^2 \right] + C_{\perp}(\nabla_z S)^2 + AS^2 + \frac{B}{2}S^4 \right\} d^3\mathbf{r},$$

C‖ >>*C*⊥

$$A(\mathbf{r}) = \alpha\left(T - T_N(\mathbf{r})\right),\quad T_N(\mathbf{r}) = T_N - \delta T_N(\mathbf{r})$$

After variation:

$$-\left[\xi_{\|}^2\left(\nabla_x^2 + \nabla_y^2\right) + \xi_z^2\nabla_z^2\right] S - \delta t(\mathbf{r})S = -t_N S.$$

$$\xi_{\|}^2 = C_{\|}/\left(aT_N\right),\ \xi_z^2 = C_{\perp}/\left(aT_N\right), \delta t(\mathbf{r}) = \frac{\delta T_N\left(\mathbf{r}\right)}{T_N}, t_N = \frac{T - T_N}{T_N}.$$

Calculations

$$H_0 = -\left[\xi_{||}^2\left(\nabla_x^2 + \nabla_y^2\right) + \xi_z^2 \nabla_z^2\right]$$

The second-order correction to dimensionless Neel temperature:

$$\langle t_{\mathrm{N}}^{(2)} \rangle = \frac{1}{V} \int \langle \delta t(\mathbf{r})\, \delta t(\mathbf{r}') \rangle G(\mathbf{r} - \mathbf{r}')\, d^3\mathbf{r}\, d^3\mathbf{r}'$$

$G(\mathbf{r}'\text{-}\mathbf{r})$ is a Green's function of the operator H_0.

Correlation function:

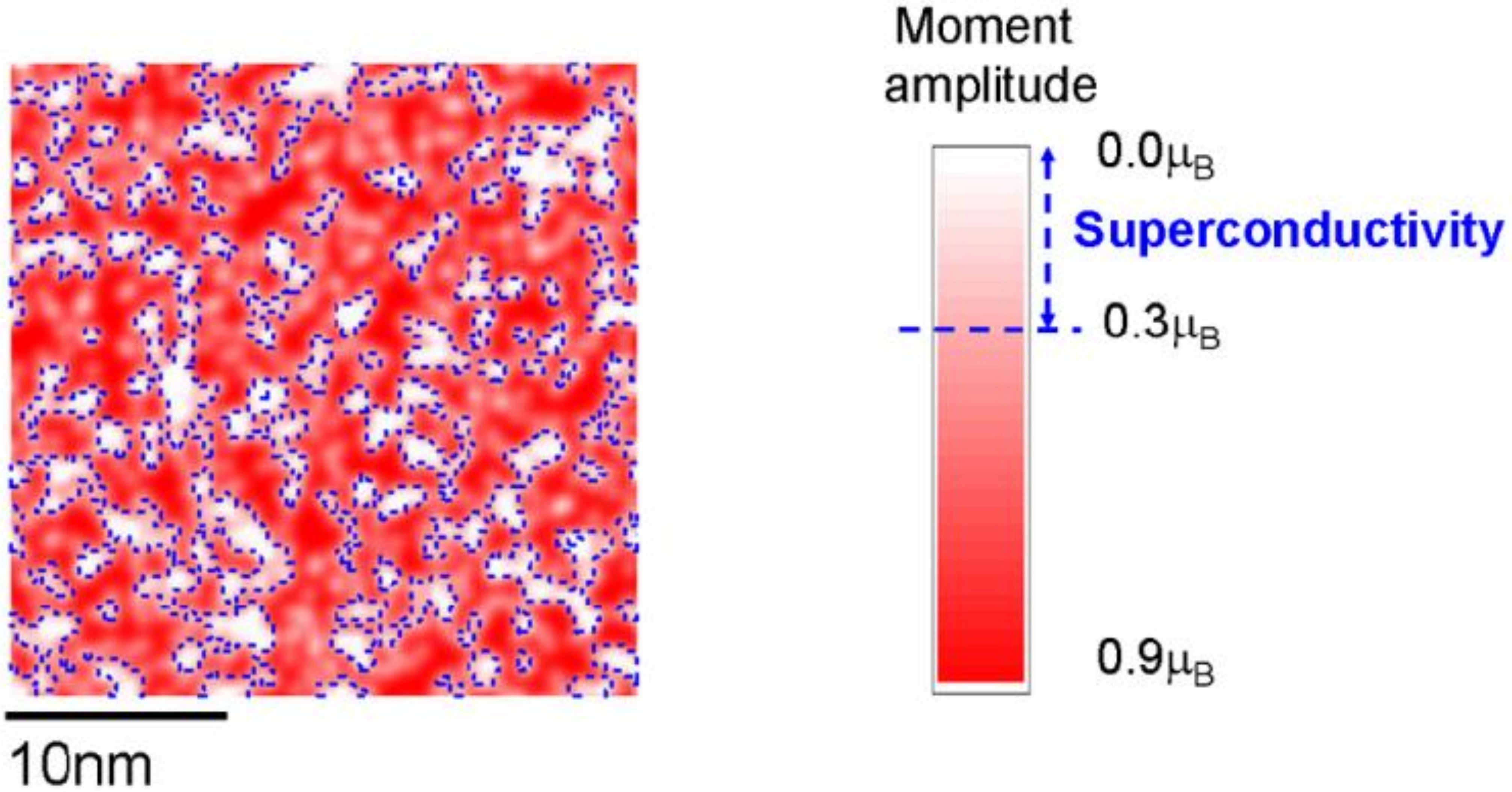
$$\tau(\mathbf{r} - \mathbf{r}') = \langle \delta t(\mathbf{r})\, \delta t(\mathbf{r}') \rangle, \tau(\mathbf{r}) = \langle \Delta t^2 \rangle \exp\left(-\frac{x^2 + y^2}{2r_0^2}\right) \delta\left(\frac{z}{s}\right)$$

Calculations

The correction to Neel temperature caused by spatial disorder:

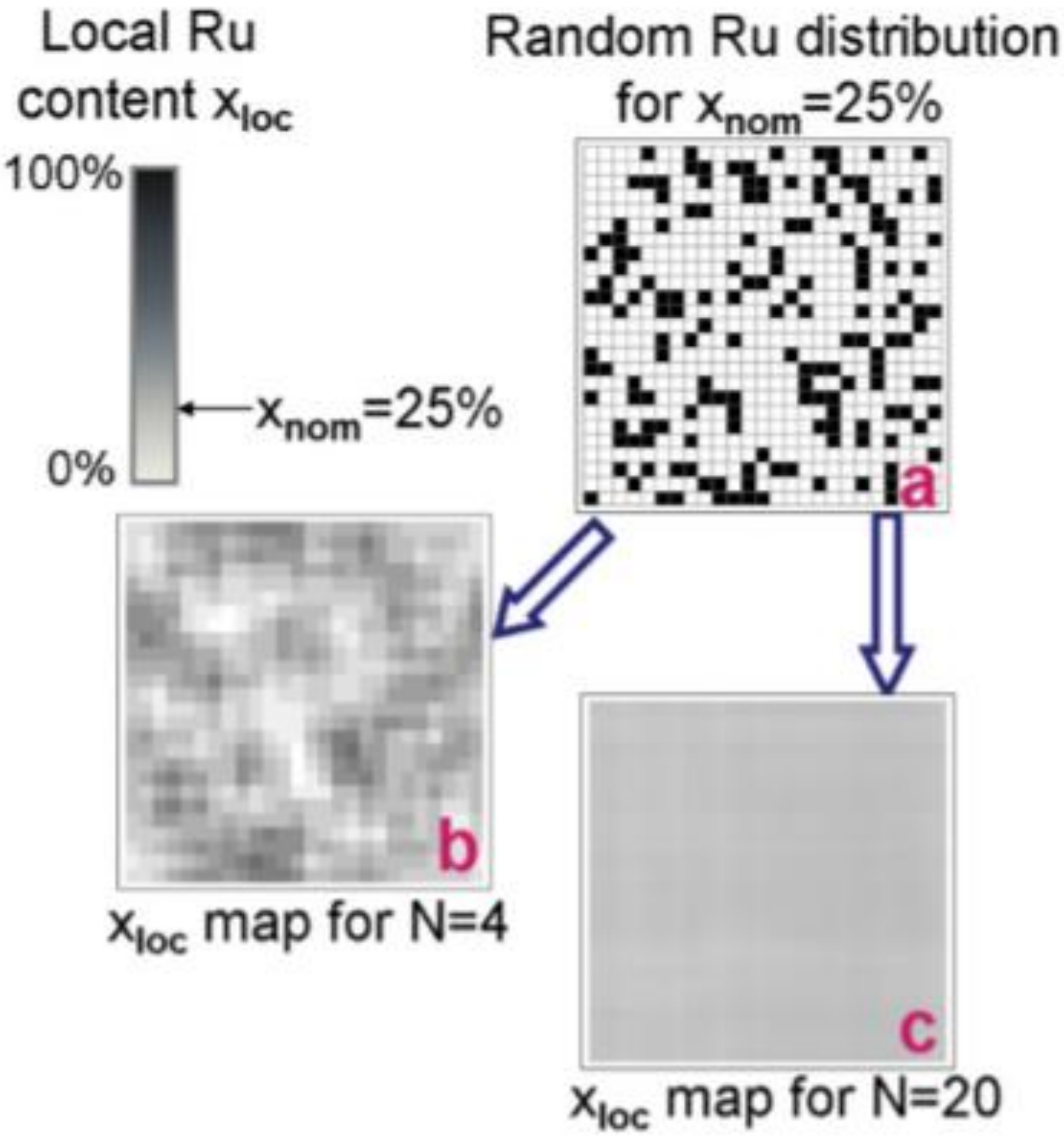
$$\langle t_{\mathrm{N}}^{(2)} \rangle \sim \frac{r_0^2}{\xi_{\|}^2} \langle \Delta t^2 \rangle$$

Analysis of experimental data



Y. Laplace, J. Bobroff, V. Brouet, G. Collin, F. RullierAlbenque, D. Colson, and A. Forget, Phys. Rev. B **86**, 020510 (2012).

Analysis of experimental data



$n(\mathbf{r})$

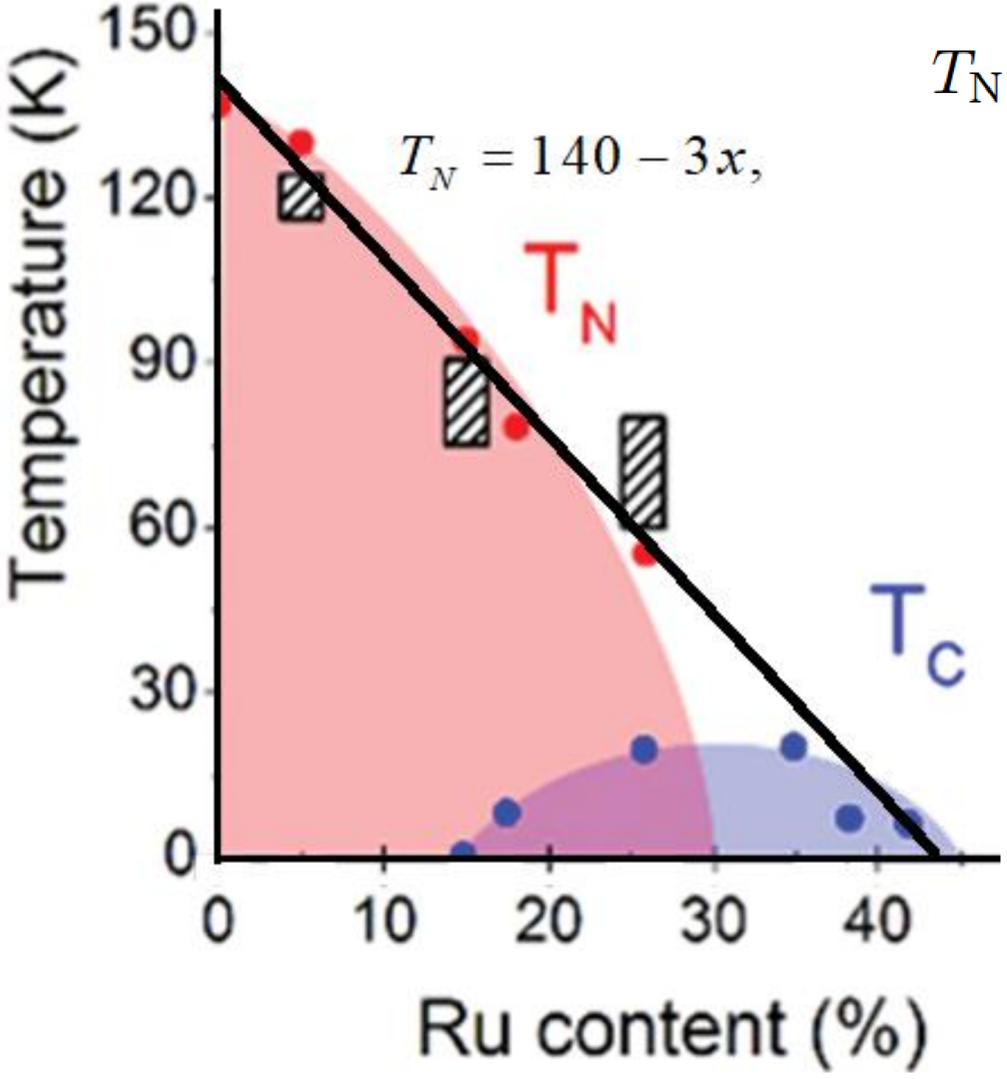
$x_{loc}(\mathbf{r}) = n(\mathbf{r})/N$

$$\langle x_{\rm loc}(\mathbf{r})\rangle = x$$

$$r_0 \approx 4a_0 \approx 11\,\text{Å}$$

Y. Laplace, J. Bobroff, V. Brouet, G. Collin, F. RullierAlbenque, D. Colson, and A. Forget, Phys. Rev. B **86**, 020510 (2012).

Analysis of experimental data



$$T_{\mathrm{N}}(x) = T_{\mathrm{N}}^{0}(1-\gamma x), \text{ where } T_{\mathrm{N}}^{0} = 140\,\mathrm{K}, \;\; \gamma = 2$$

$$\delta t(\mathbf{r}) = \frac{\gamma\,(n - n(\mathbf{r}))}{N - \gamma n}$$

$$\langle \Delta t^2 \rangle = \frac{\gamma^2 \langle \Delta n^2 \rangle}{(N-\gamma n)^2}, \quad \text{where} \quad \Delta n = n(\mathbf{r}) - n$$

$$\langle \Delta n^2 \rangle = n(N-n)/N$$

Y. Laplace, J. Bobroff, V. Brouet, G. Collin, F. RullierAlbenque, D. Colson, and A. Forget, Phys. Rev. B **86**, 020510 (2012).

Analysis of experimental data

The correction to Neel temperature in Kelvin:

$$\Delta T_{\mathrm{N}} \approx \frac{r_0^2 \gamma^2 n(N-n)}{\xi_{\|}^2 N^2 (N-\gamma n)} T_{\mathrm{N}}^0$$

$$\Delta T_{\mathrm{N}} \approx \frac{a_0^2 \gamma^2 x(1-x)}{\xi_{\|}^2 (1-\gamma x)} T_{\mathrm{N}}^0$$

Analysis of experimental data

Estimation $\xi_{||}$ from the microscopic BCS-like theory:

$$\xi_{||}(x) \approx \frac{0.13\, v_{\mathrm{F}}}{T_{\mathrm{N}}} \approx \frac{0.13\, v_{\mathrm{F}}}{T_{\mathrm{N}}^{0}(1-\gamma x)}$$

$$v_{\mathrm{F}} \sim 0.7\, \mathrm{eV\AA}$$

$$\Delta T_{\mathrm{N}} \approx \frac{a_0^2 \gamma^2 x(1-x)\,(1-\gamma x)}{(0.13 v_{\mathrm{F}})^2} (T_{\mathrm{N}}^{0})^3$$

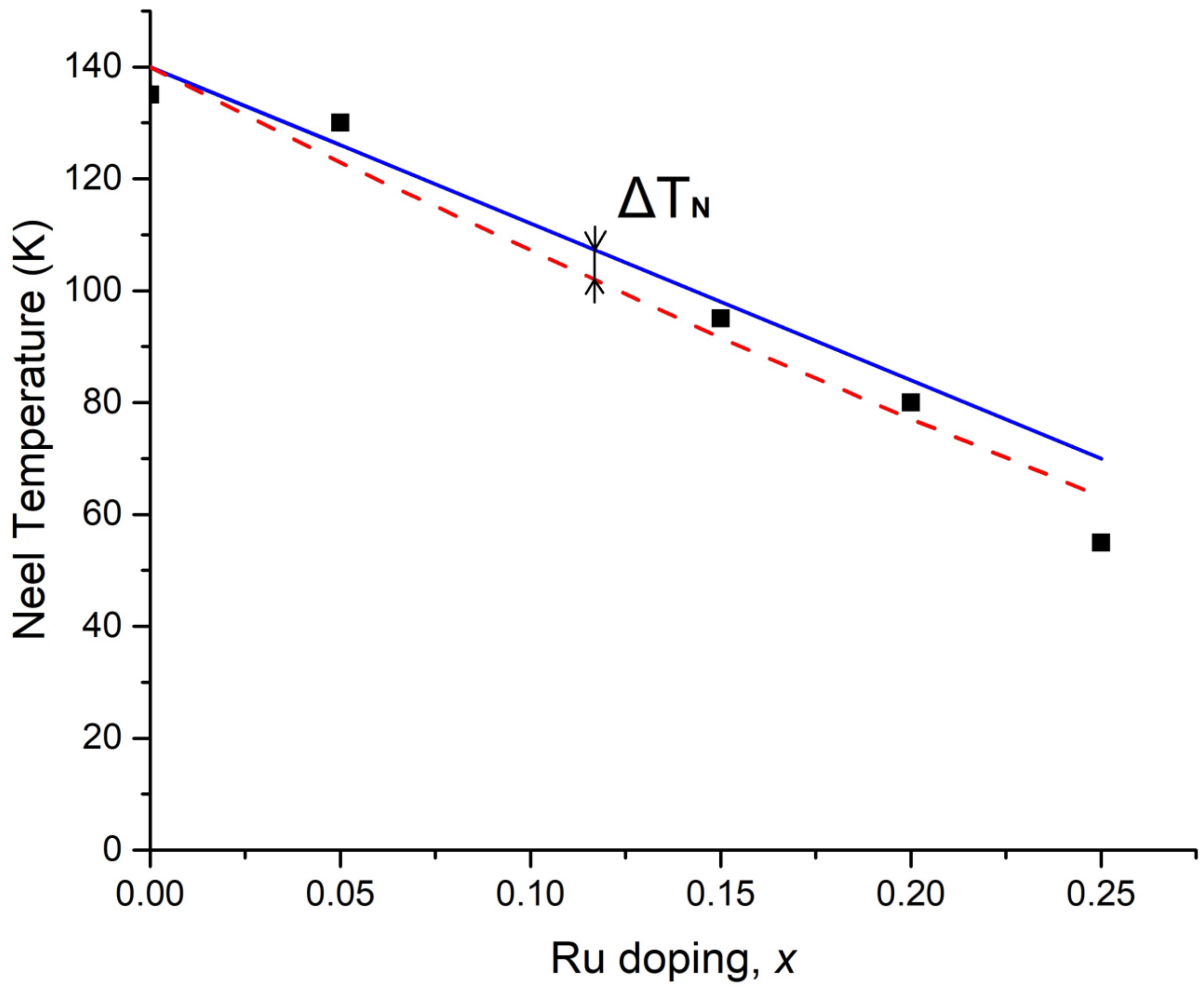
R. S. Dhaka, et al., Phys. Rev. Lett. **107**, 267002 (2011).

Analysis of experimental data

The correction to Neel temperature:

$$\Delta T_{\mathrm{N}} \approx 74x(1-x)\,(1-2x)$$

The correction to Neel temperature



Summary

- Using the perturbation theory, we calculated the correction to the Neel temperature of a quasi-two-dimensional system.
- The derived formula was applied to the analysis of data for Rudoped $BaFe_2As_2$.
- It was demonstrated that the correction is quite small for all doping levels where the material demonstrates the SDW transition.
- This suggests that the Neel temperature in Ru-doped $BaFe_2As_2$ may be studied using spatially homogeneous models, disregarding disorder.