Metal - Mott insulator heterostructures: real space dynamical mean-field study

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INNOVATIVE ECONOMY
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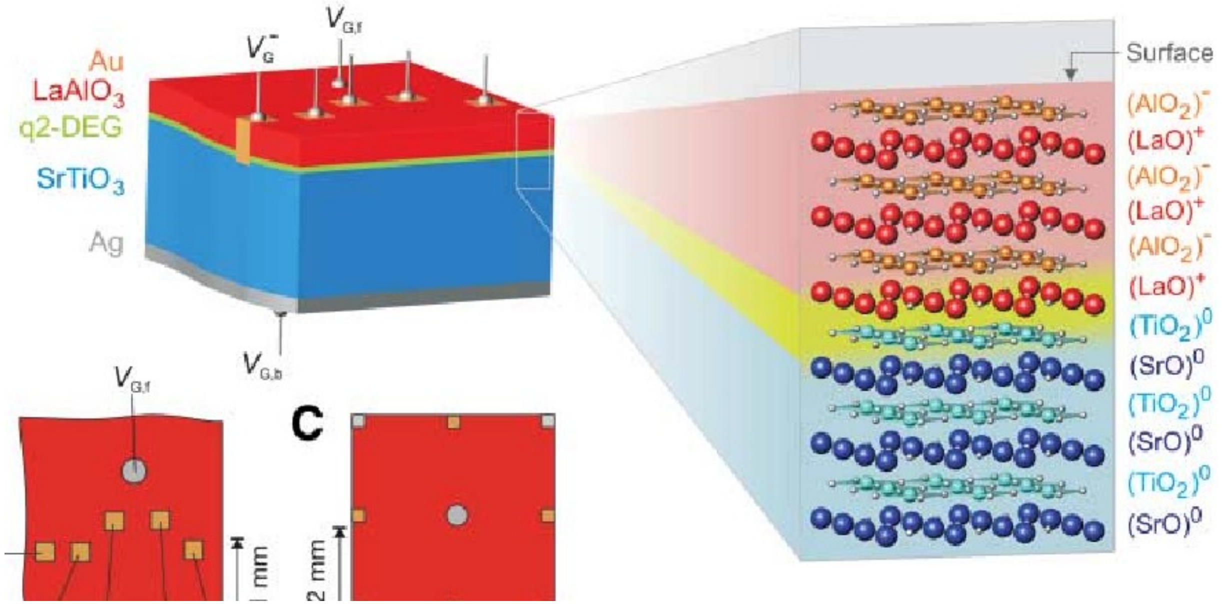
Motivation

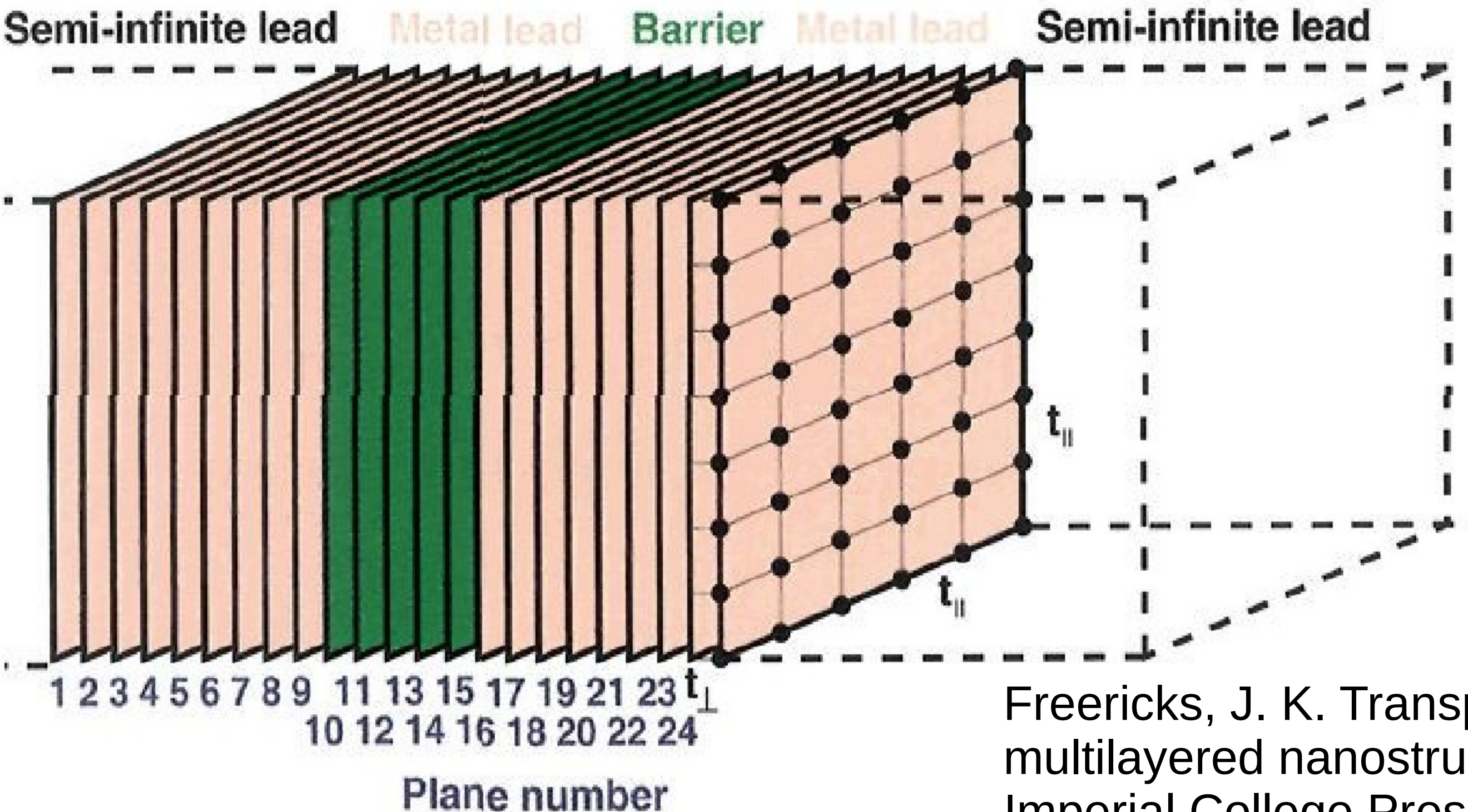
Experiment: phenomena observed at the interface of two materials can be different than those seen in the bulk.

Oxide heterostructures: two-dimensional electron gases can appear at the interfaces of band and Mott insulator.



S. Thiel et al., Science 313, 1942 (2006)

Goal of our research: proximity effects in metal – Mott insulator – metal heterostructure



Freericks, J. K. Transport in multilayered nanostructures, Imperial College Press, 2006

Electronic properties in the heterostructure; in particular:

-density of states (at the Fermi level), double occupation number, internal energy,...

Model of metal – Mott insulator – metal heterostructure

One-band Hubbard model in an infinite simple cubic lattice:

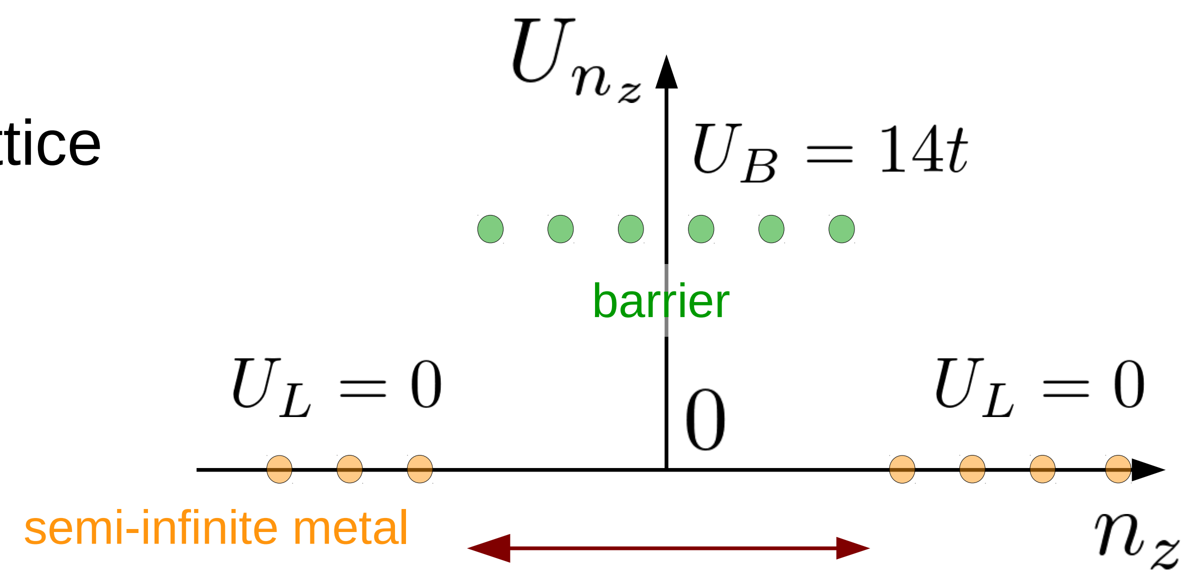
$$H = \sum_{(\mathbf{i},\mathbf{j})\in n.n.} \sum_{\sigma=\uparrow,\downarrow} t_{\mathbf{ij}} \hat{c}^{\dagger}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{i}\sigma} + \sum_{\mathbf{i}} U_{\mathbf{i}} \hat{n}_{\mathbf{i}\uparrow} \hat{n}_{\mathbf{i}\downarrow} - \sum_{\mathbf{i}} \sum_{\sigma=\uparrow,\downarrow} \mu_{\mathbf{i}} \hat{n}_{\mathbf{i}\sigma}$$

$$\hat{n}_{i\sigma} \equiv \hat{c}^{\dagger}_{i\sigma} \hat{c}_{i\sigma}$$

-uniform hopping in all directions

$$t_{\mathbf{ij}} = -t$$

-interaction depends on lattice site in the heterostructure (translational symmetry in x and y direction)



width of Mott insulator
(in the picture 6 lattice sites)

-assumed half-filling

$$\mu_{\mathbf{i}} = \frac{U_{\mathbf{i}}}{2}$$

-spin symmetry (paramagnetic state)

Different approximations

Gupta, S. & Gupta, T. Solid State Communications, 2012, 152, 53-5, T=0, Hartree-Fock

G. Borghi, M. Fabrizio, E. Tosatti, Physical Review B, vol. 81, no. 11, p. 115134, 2010, T=0,
self-consistent Gutzwiller technique

M. Potthof and W. Nolting, Physical Review B, vol. 59, no. 4, p. 2549, 1999, T=0, DMFT, ED
M. Potthof and W. Nolting, Physical Review B, vol. 60, no. 11, p. 7834, 1999. T=0, L-DMFT, ED

Okamoto, Satoshi and Millis, Andrew J, Physical Review B, vol. 70, no. 24, p. 241104, 2004, dif model with Coulomb, two-site DMFT

Helmes, R.; Costi, T. & Rosch, A. Physical review letters, 2008, 101, 066802; T=0, NRG

H. Zenia, J. K. Freericks, H. R. Krishnamurthy, and Th. Pruschke Physical review letters 2009, 103, 116402. NRG

Ishida, H., and A. Liebsch. Physical Review B 79.4 (2009): 045130, finite temp. ED

Our approch: DMFT without further approximations (i.e. ctqmc algorithm)

Dynamical Mean Field Theory

- *W. Metzner, D. Vollhardt, Phys. Rev. Lett. 59, 121 (1987)*
- *A. Georges, G. Kotliar, W. Krauth, M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996)*
- *M. Potthoff, W. Nolting, Phys. Rev. B, 1999, 59, 2549*
- *Freericks, J. K. Transport in multilayered nanostructures, Imperial College Press, 2006*

Quasi 1d Dyson equation for Green function:

$$\left(i\omega_n + \mu_\alpha - \varepsilon^{||} - \Sigma_\alpha\left(i\omega_n\right)\right) G_{\alpha\beta}\left(i\omega_n, \varepsilon^{||}\right) + t^{1D}_{\alpha\alpha+1} G_{\alpha+1\beta}\left(i\omega_n, \varepsilon^{||}\right) + t^{1D}_{\alpha\alpha-1} G_{\alpha-1\beta}\left(i\omega_n, \varepsilon^{||}\right) = \delta_{\alpha\beta}$$

Local Dyson equation:

$$\Delta_\alpha\left(i\omega_n\right) = i\omega_n + \mu - \frac{1}{G_{\alpha\alpha}\left(i\omega_n\right)} - \Sigma_\sigma\left(i\omega_n\right)$$

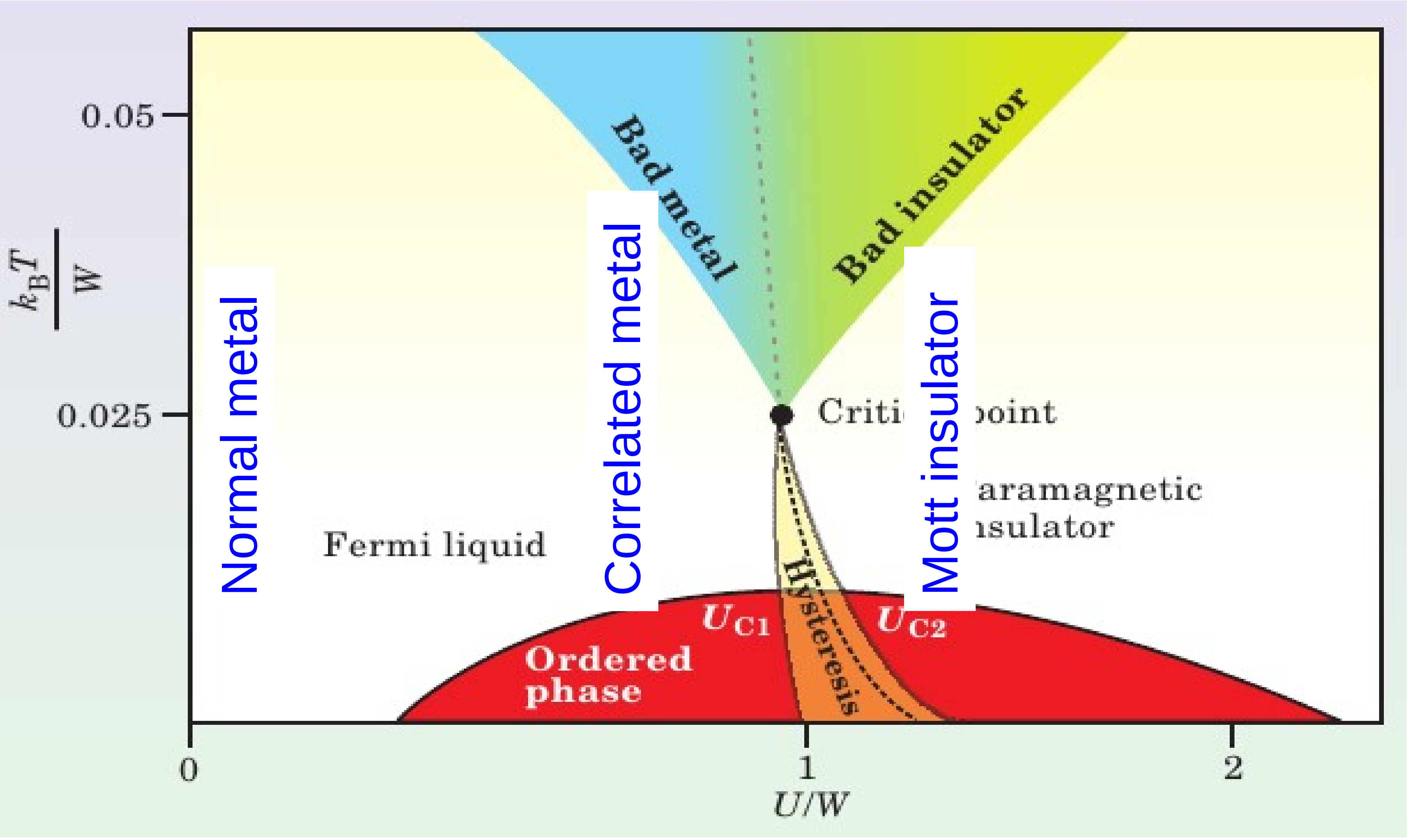
Single impurity problem: $G_{\alpha\alpha}(\tau,\tau') = -\langle c_{0\sigma}(\tau) c^*_{0\sigma}(\tau')\rangle_{S_{\text{eff}}[\Delta_\alpha]}$

Anderson, P. W. (1961). Phys. Rev., 124, 41

(solved by our continuous time Monte Carlo algorithm – hybridization expansion)

Hirsch, J. E., and R. M. Fye, Phys. Rev. Lett. 56, 2521 (1986,)
Continuous time: Prokof’ev, N. V., and B. V. Svistunov, 1998, Phys. Rev. Lett. 81, 2514
Gull et al. Rev Mod Phys 83, 349 (2011)

Hubbard Model for bulk materials – schematic phase diagram



Kotliar and Vollhardt, Phys. Today 57, 53-60 (2004)

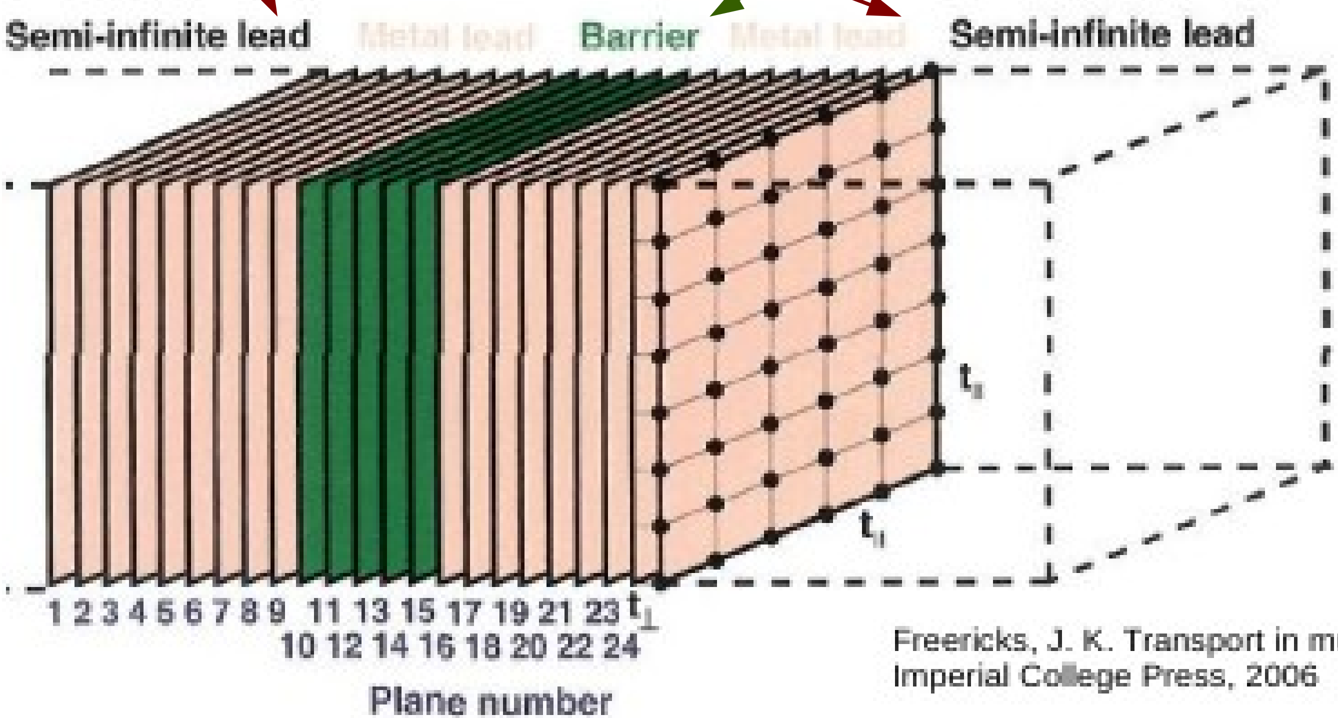
Critical point
(paramagnetic, our results):

$$k_B T_c \approx 0.1t \approx 0.083W$$
$$U_c(T_c) \approx 11.3t$$

Results Example of determination of coexistence region

Interaction in semi-infinite leads: $U_L = 0$

Interaction in Barrier: $U_B = 14t \quad > U_c(T_c)$



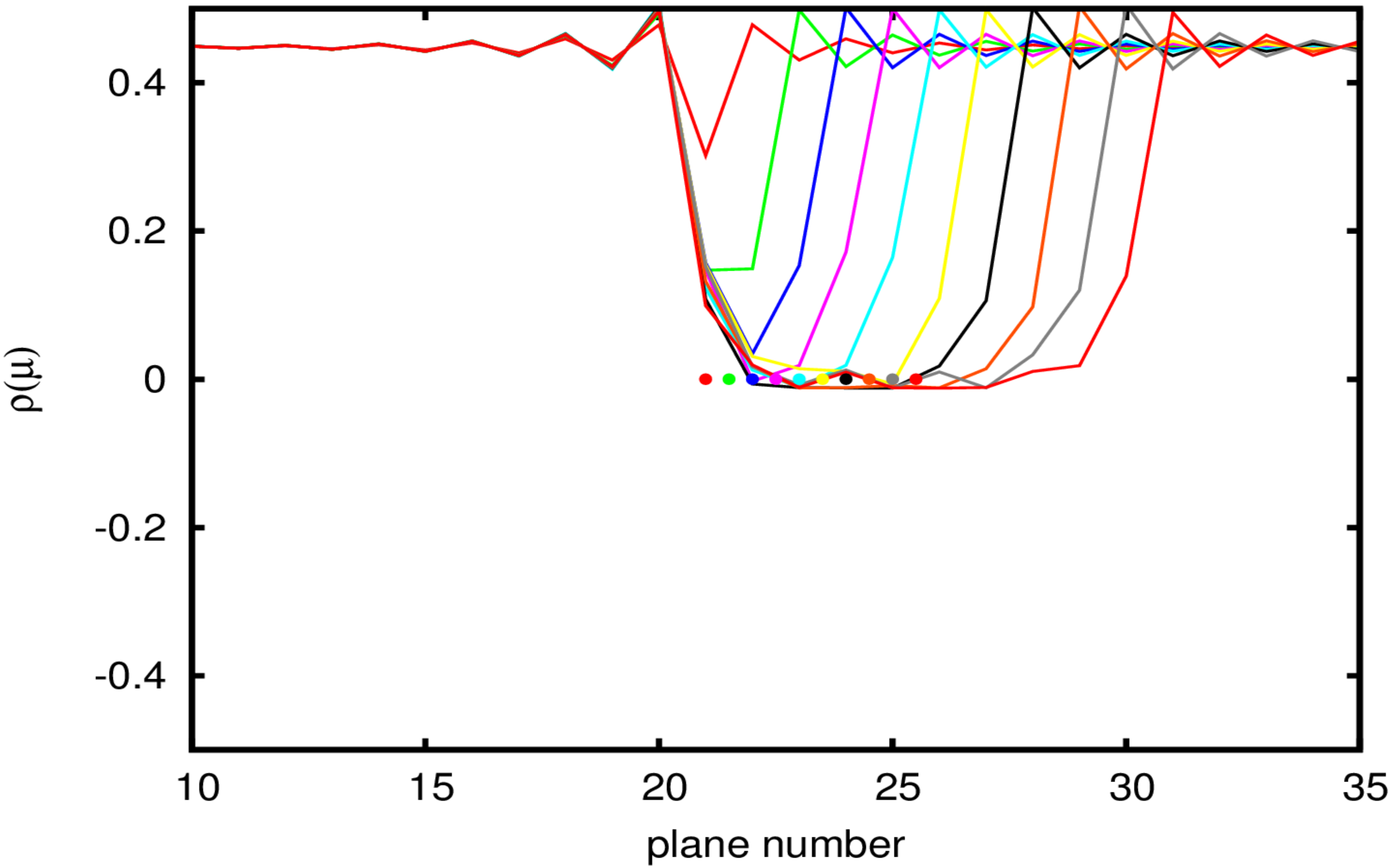
Freericks, J. K. Transport in multilayered nanostructures, Imperial College Press, 2006

Number of insulator layers: $1, 2, 3, \ldots, 9, 10$

Different temperatures: $\beta t = 1, 2, 4, 8, 16, 32$

Density of states at the Fermi level in heterostructure

$U_L = 0$ $U_B = 14t$ $U_L = 0$



$\beta = 16t$

Density of states at the Fermi level in heterostructure

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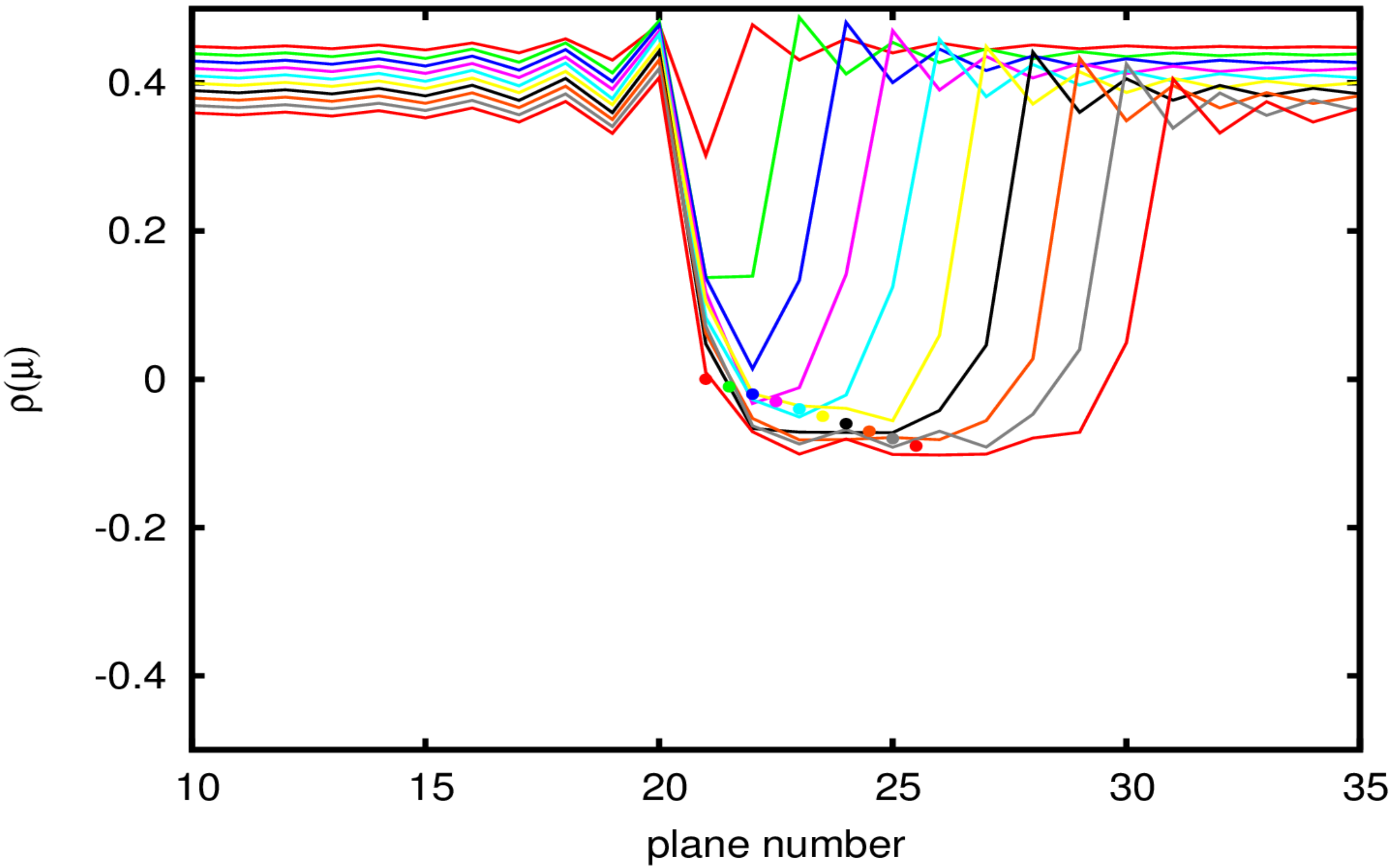

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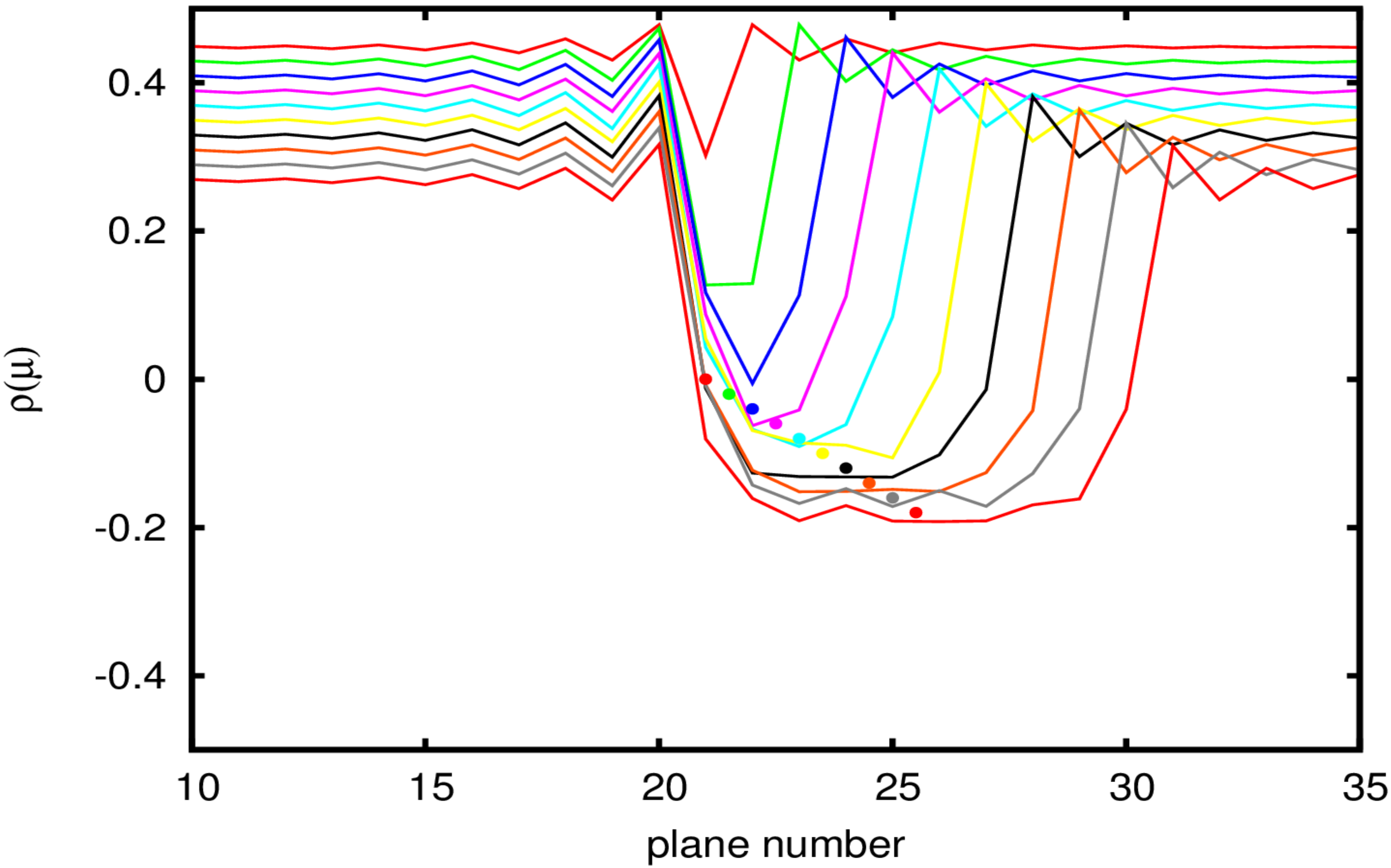

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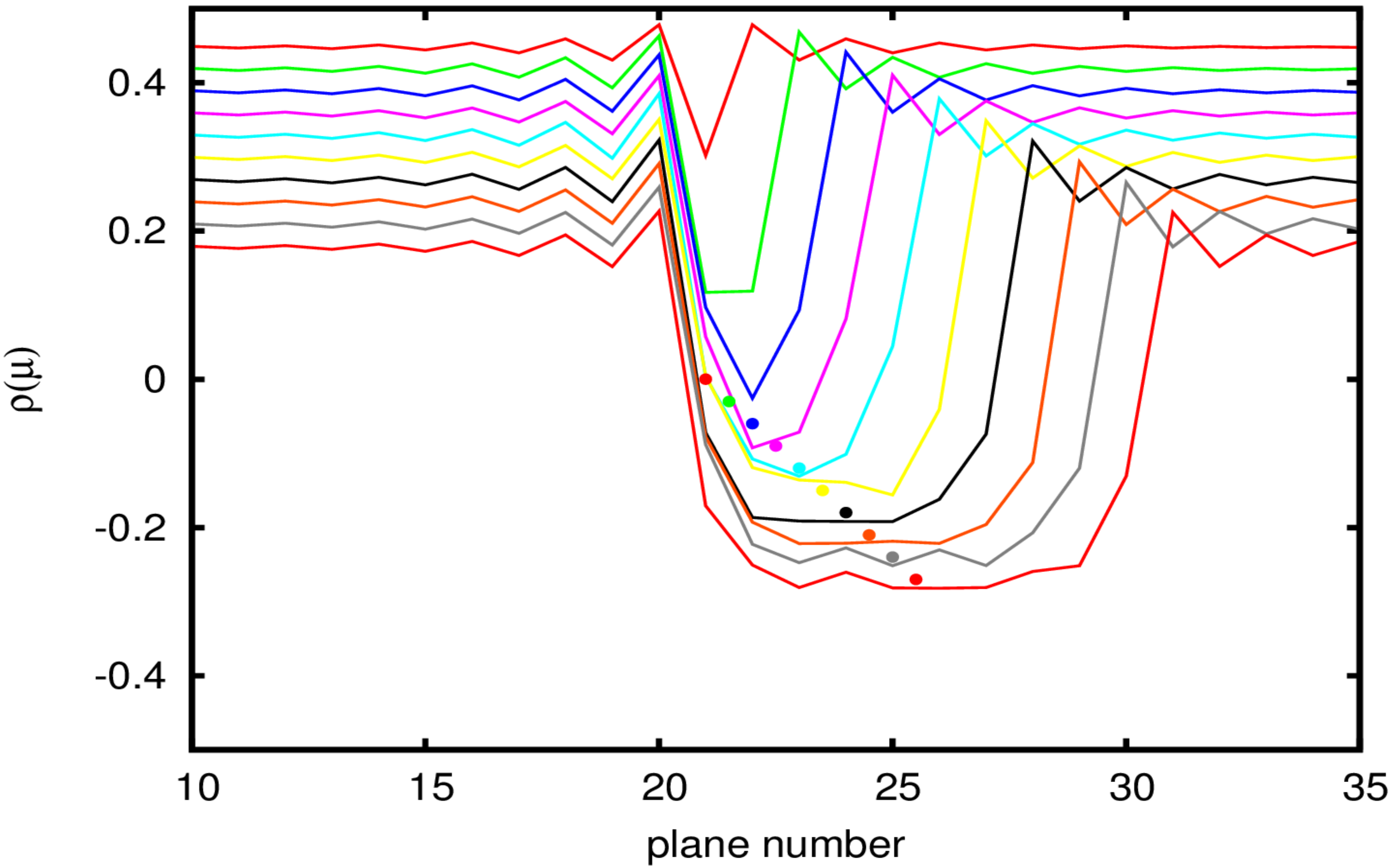

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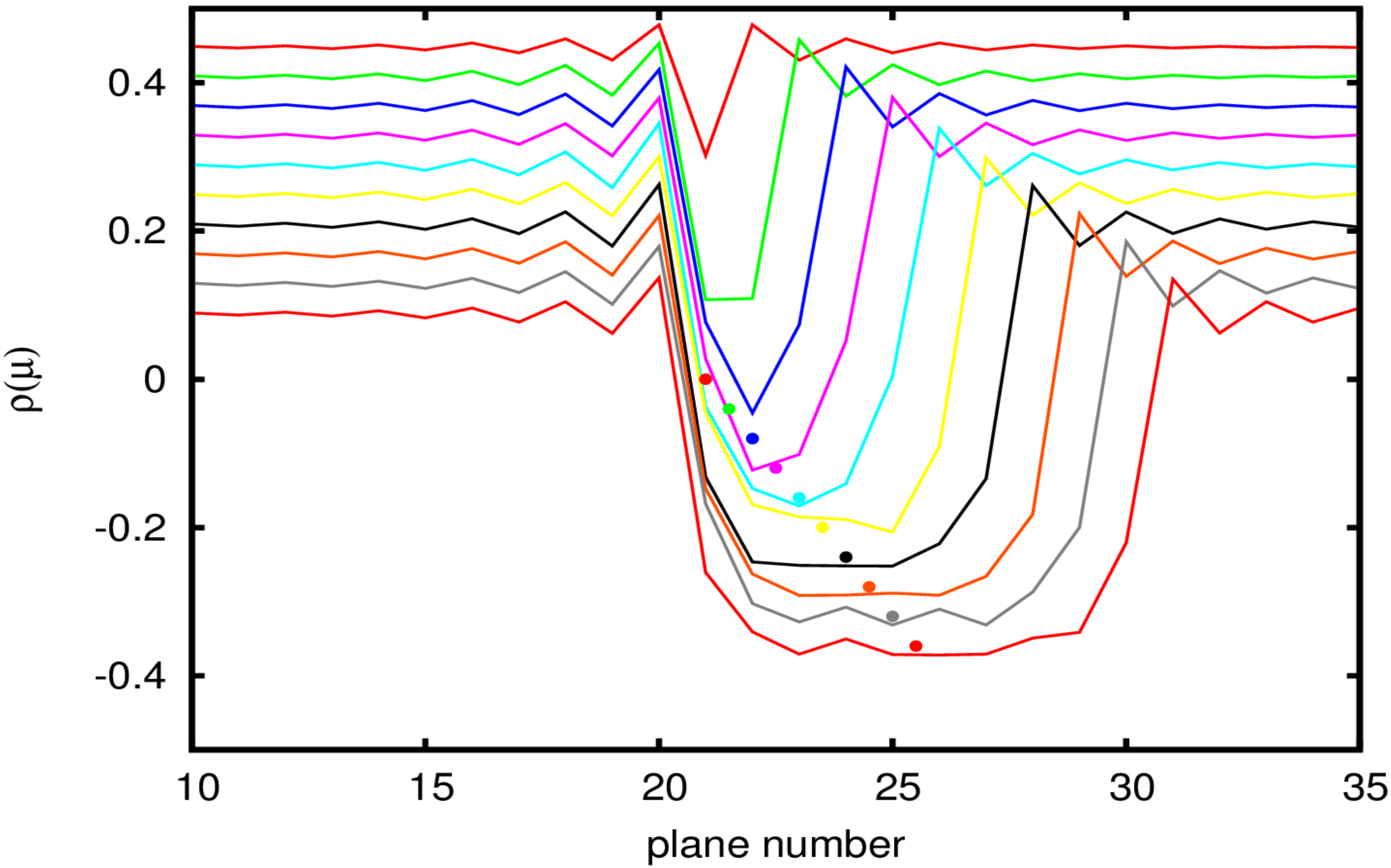

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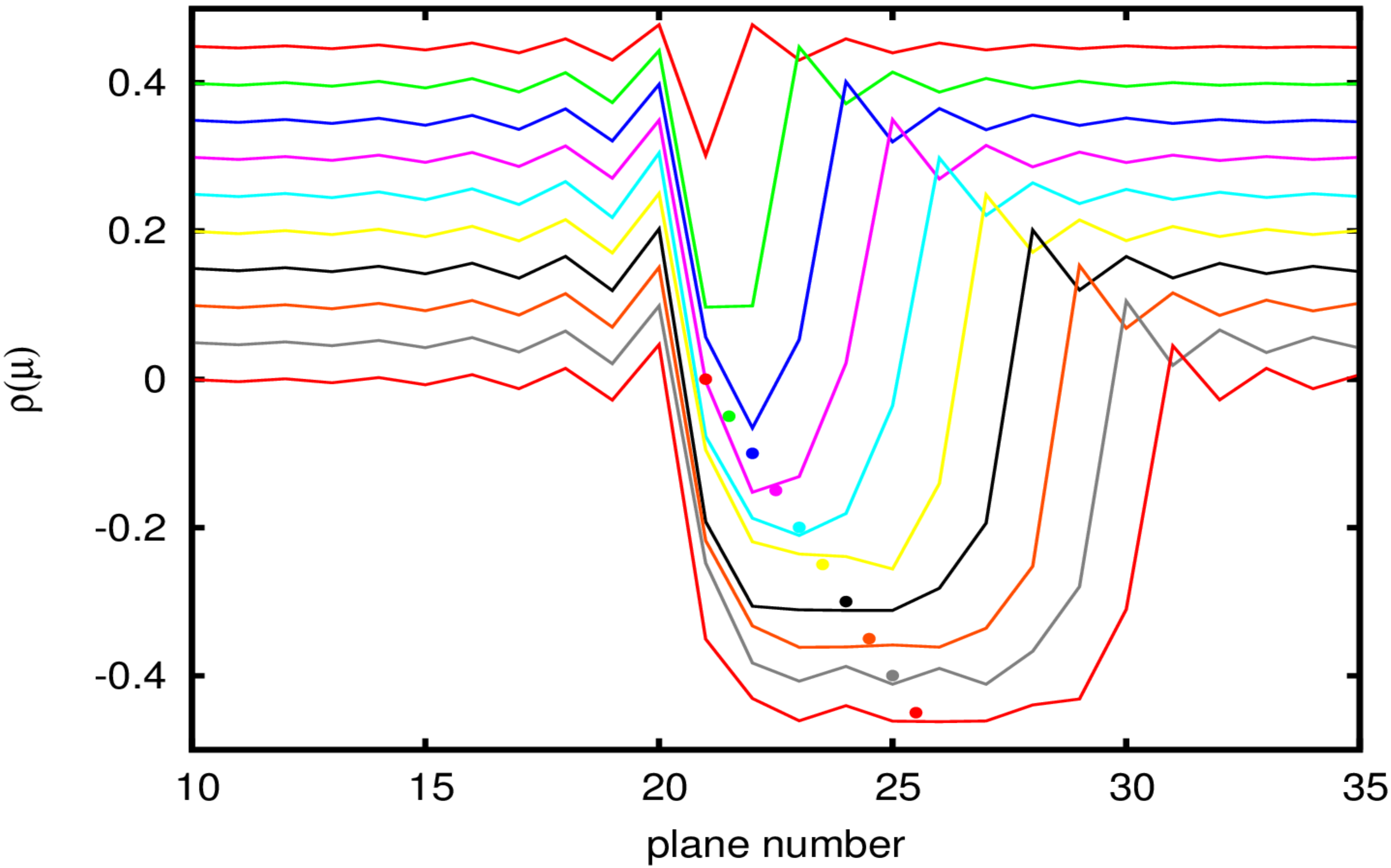
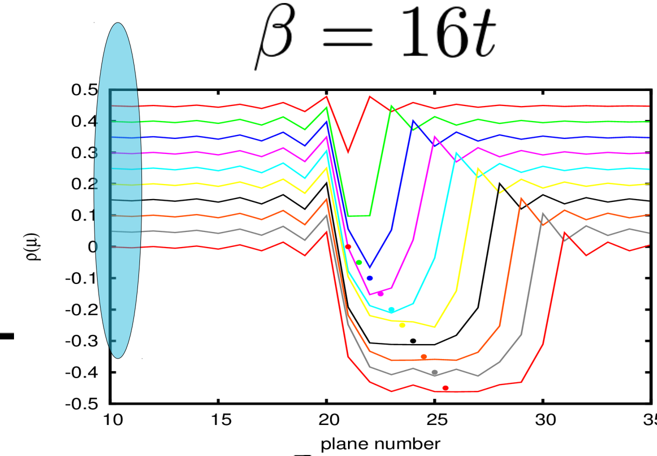


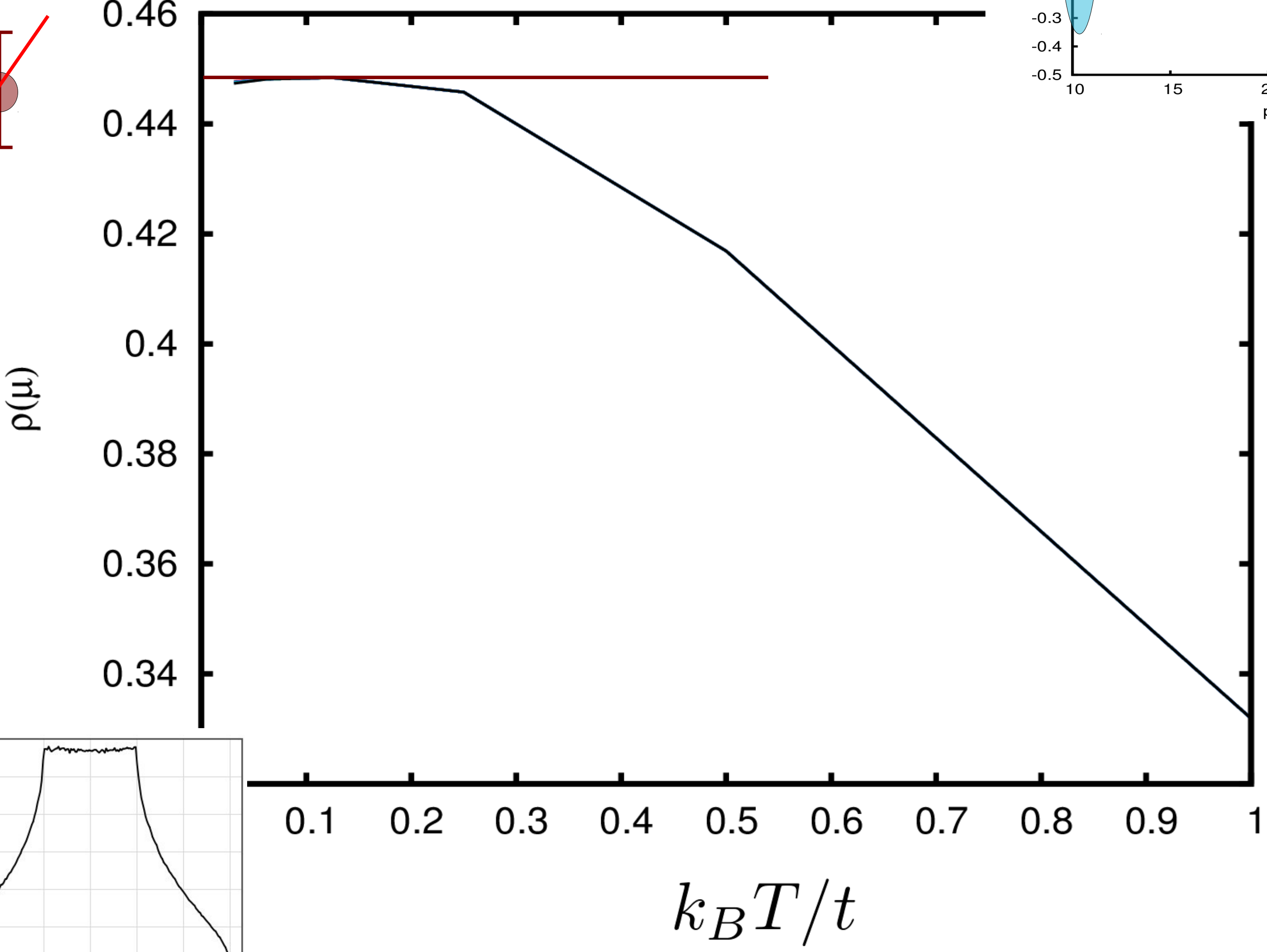
$\beta = 16t$

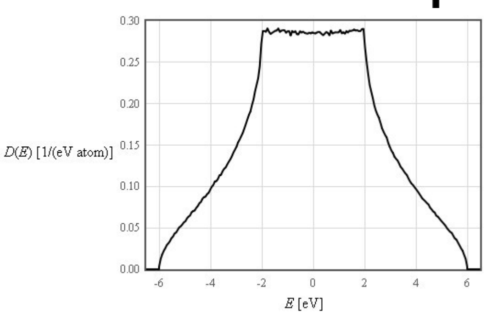
Density of states in the bulk

$$\rho(\mu) \sim \lim_{\beta\to\infty} \beta G(\beta/2)$$

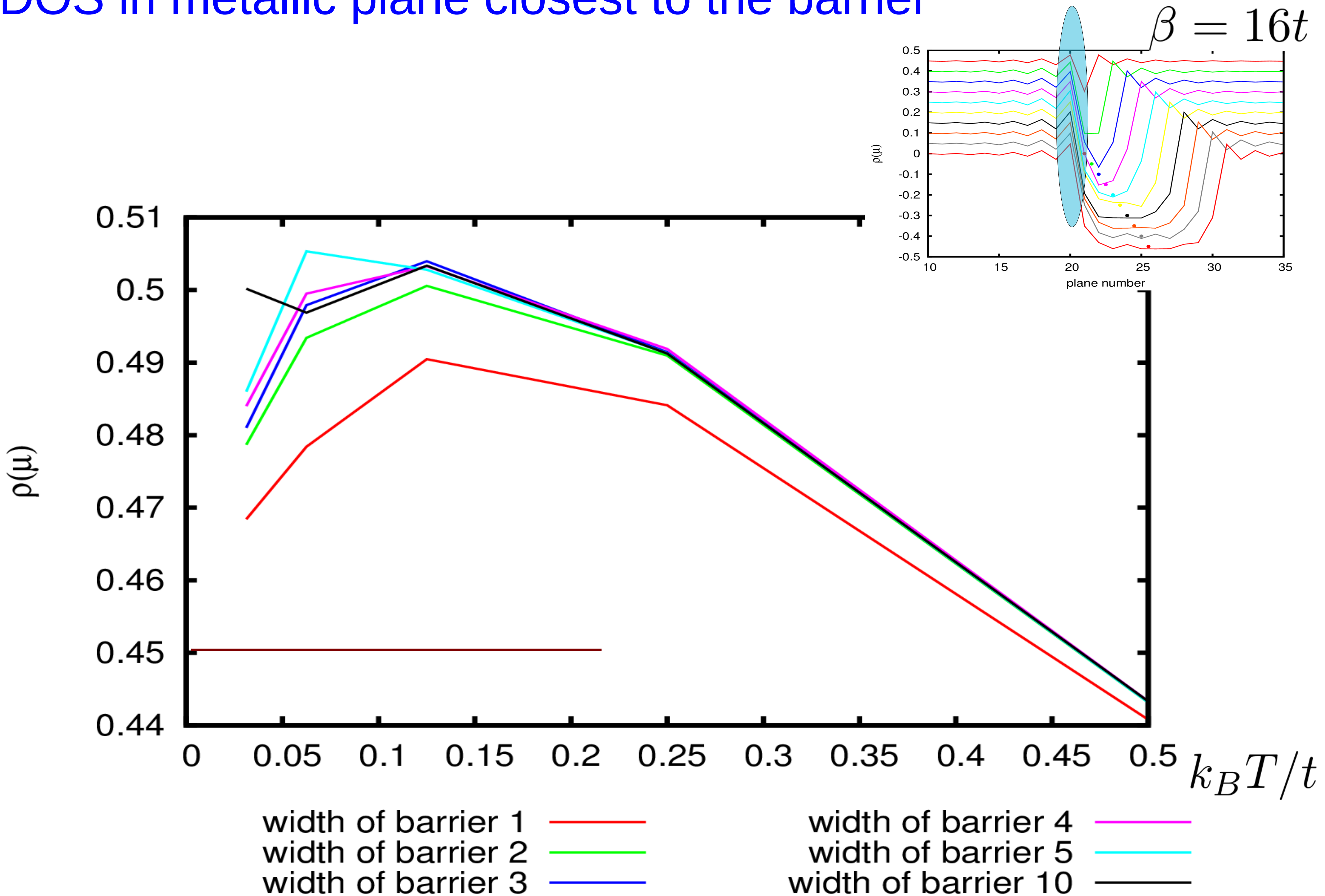
$\beta = 16t$





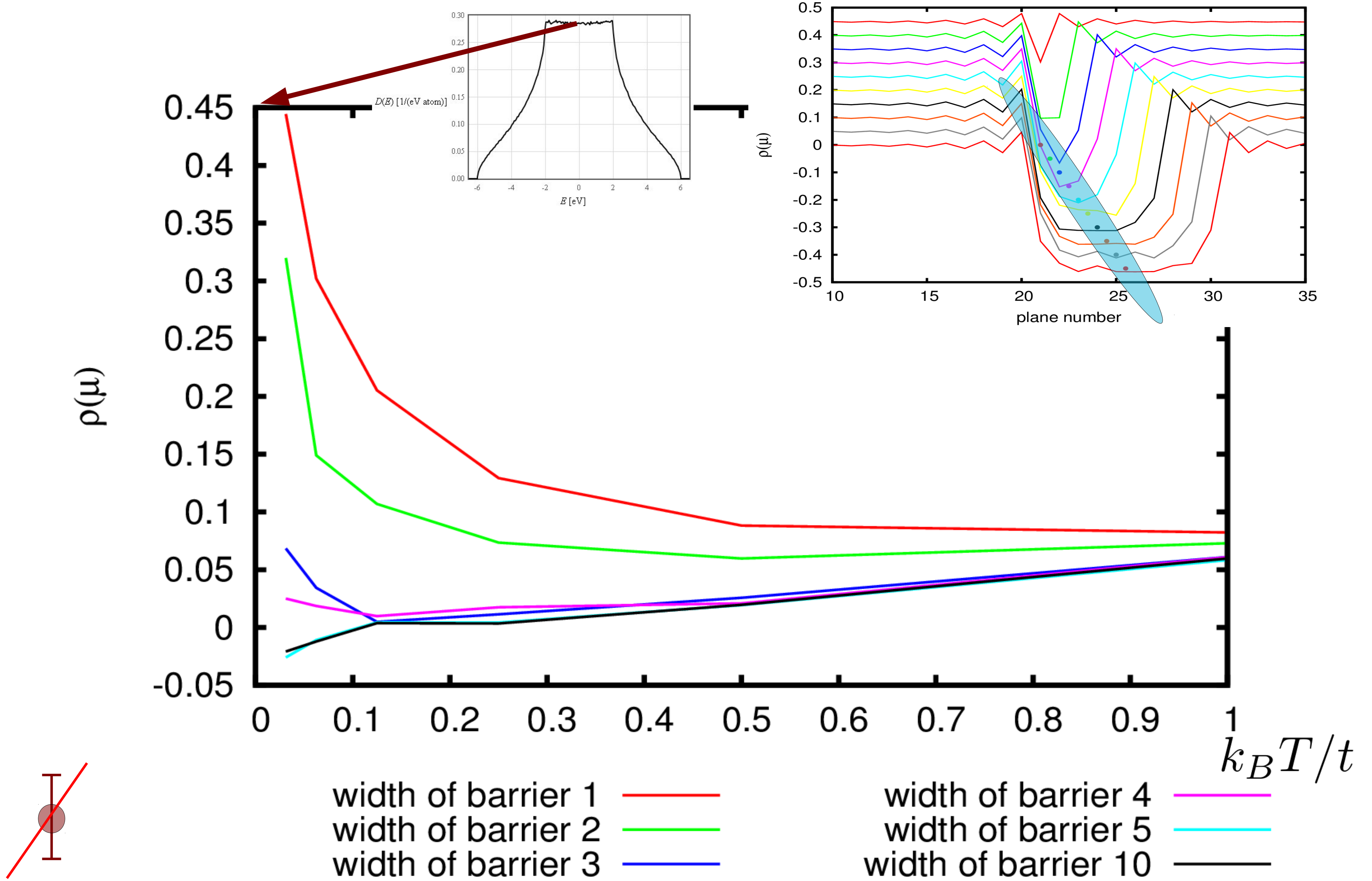


DOS in metallic plane closest to the barrier



DOS in the middle of heterostructure

$\beta = 16t$



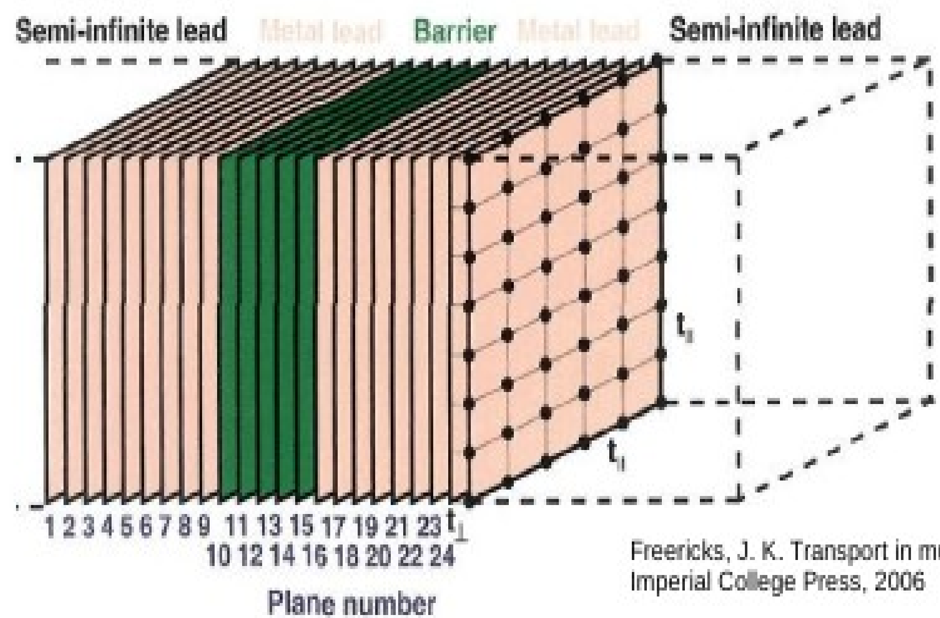
Summary

Metal – Mott insulator – metal heterostructure
One-band Hubbard model within DMFT with ctqmc algorithm (without further approximations)

Proximity effect in metal – Mott insulator – metal heterostructure (density of states at Fermi level)

-the most metallic is a layer in lead which is closest to the barrier (oscillations in metal)

-monotonic change of DOS in the barrier



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