Metal - Mott insulator heterostructures: A dynamical mean field study

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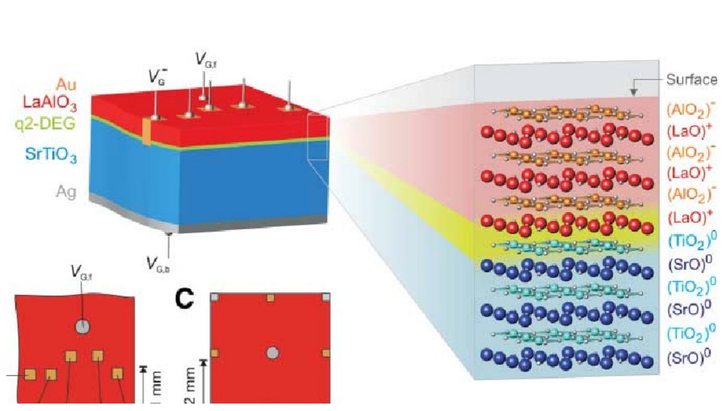
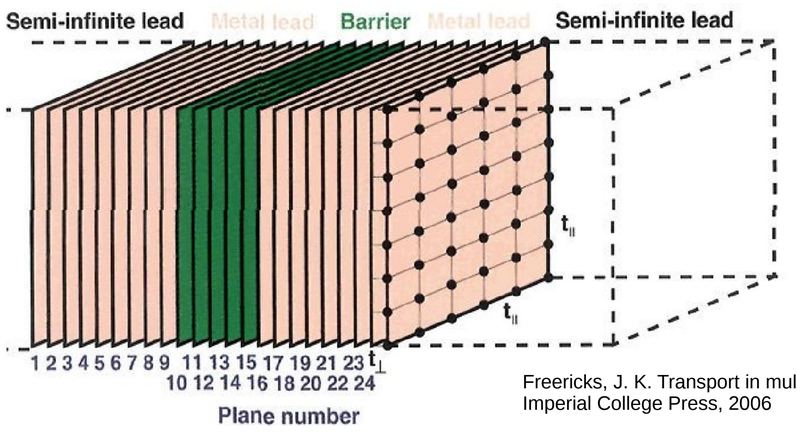
Motivation and aims

Phenomena observed at the interface of two materials can be different than those seen in the bulk. For example, in oxide heterostructures two-dimensional electron gases can appear at the interfaces of band and Mott insulator.



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

We consider three dimensional heterostructure consisted of Mott insulator (green colour below) between two semi-infinite band insulators



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

Our aim is to calculate electronic properties in the heterostructure. In particular:
- -quasi particle density of states
- -average kinetic energy of particles
- -double occupation number

which depend on the position in the heterostructure.

Model of the heterostructure

The system under consideration is described by grand canonical Hamiltonian of one band Hubbard model:

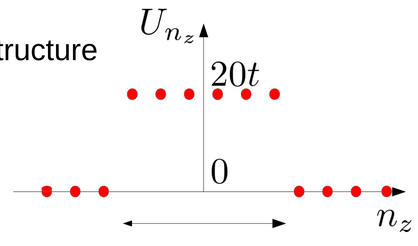
$$H = \sum_{(\mathbf{i},\mathbf{j})\in n.n.} \sum_{\sigma=\uparrow,\downarrow} t_{\mathbf{ij}} \hat{c}^{\dagger}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{i}\sigma} + \sum_{\mathbf{i}} U_{\mathbf{i}} \hat{n}_{\mathbf{i}\uparrow} \hat{n}_{\mathbf{i}\downarrow} - \sum_{\mathbf{i}} \sum_{\sigma=\uparrow,\downarrow}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

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

for infinite simple cubic lattice

$$\mathbf{j}, \mathbf{i} \in [n_x \hat{\mathbf{e}}_x, n_y \hat{\mathbf{e}}_y, n_z \hat{\mathbf{e}}_z] \qquad n_x, n_y, n_z = \ldots, -1, 0, 1, \ldots$$

with the following properties
- -uniform hopping in all directions: $t_{\mathbf{ij}} = t$
- -assumed half-filling $\mu_{\mathbf{i}} = \frac{U_{\mathbf{i}}}{2}$
- -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)

Method: dynamical mean field theory

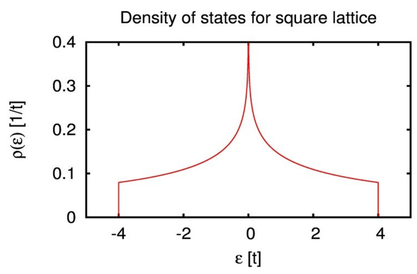
- *W. Metzner, D. Vollhardt, Phys. Rev. Lett. 59, 121 (1987)*
- *A. Georges, G. Kotliar, W. Krauth, M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996)*
- *Freericks, J. K. Transport in multilayered nanostructures, Imperial College Press, 2006*

$$G_{\mathbf{ij}}(\tau, \tau') = -\langle c_{\mathbf{i}\sigma}(\tau) \hat{c}^{\dagger}_{\mathbf{j}\sigma}(\tau') \rangle$$

Dyson equation with use of translational symmetry in x and y direction (quasi 1-dimensional system):

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

$$G_{\alpha\alpha}(i\omega_n) = \int_{-\infty}^{\infty} d\varepsilon \rho^{2d}\left(\varepsilon^{||}\right) G_{\alpha\alpha}\left(i\omega_n, \varepsilon^{||}\right)$$



Local Dyson equation:

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

Single impurity problem (solved by continuous time Monte Carlo algorithm):

$$G_{\alpha\alpha}(i\omega_n) = -\frac{1}{\Xi}\left[\prod_\sigma \int D\varphi_\sigma \int D\varphi^*_\sigma\right] \varphi_\sigma(i\omega_n)\, \varphi^*_\sigma(i\omega_n) \exp\left[-S_\alpha\right]$$

$$S_\alpha = \sum_\sigma \int_0^\beta d\tau \varphi^*_\sigma(\tau)\left(\frac{\partial}{\partial\tau} - \mu_\alpha\right)\varphi_\sigma(\tau) + U_\alpha \int_0^\beta d\tau \varphi^*_\uparrow(\tau)\varphi_\uparrow(\tau)\varphi^*_\downarrow(\tau)\varphi_\downarrow(\tau) + \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma \varphi^*_\sigma(\tau)\Delta_\alpha(\tau-\tau')\varphi_\sigma(\tau')$$

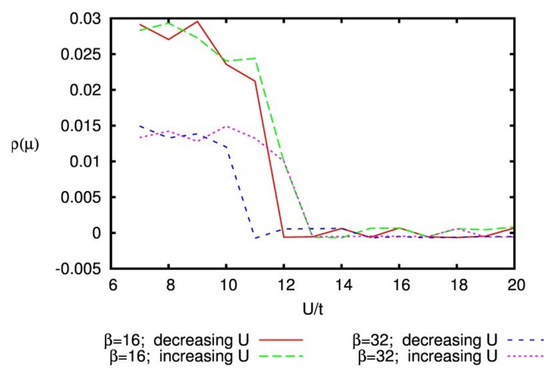
$$\beta = 1/(k_B T)$$

Results

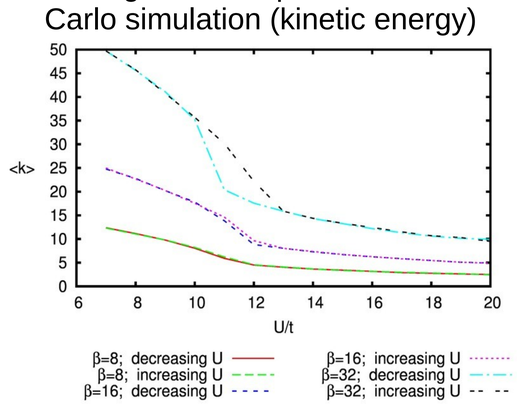
Before heterostructure - homogeneous Hubbard model

$$H = t \sum_{(\mathbf{i},\mathbf{j})\in n.n.} \sum_{\sigma=\uparrow,\downarrow} \hat{c}^{\dagger}_{\mathbf{i}\sigma} \hat{c}_{\mathbf{i}\sigma} + U \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}\uparrow} \hat{n}_{\mathbf{i}\downarrow} - \mu \sum_{\mathbf{i}} \sum_{\sigma=\uparrow,\downarrow} \hat{n}_{\mathbf{i}\sigma}$$

Density of states (at chemical potential)



Average order expansion in Monte Carlo simulation (kinetic energy)



$$G(\tau) = \int_{-\infty}^{\infty} d\omega \rho(\omega) \frac{e^{-(\omega-\mu)\tau}}{1 + e^{-(\omega-\mu)\beta}}$$

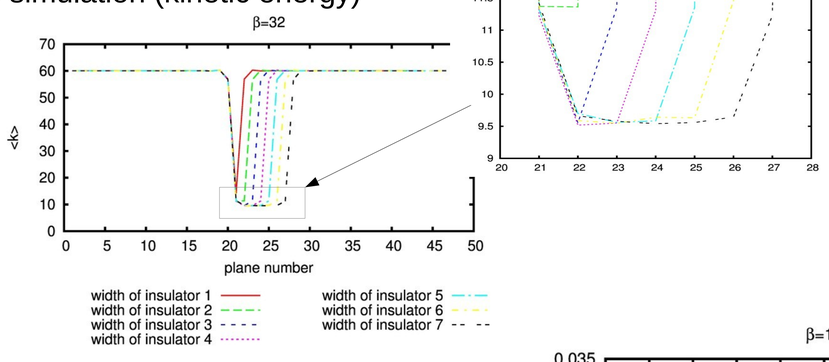
Kinetic energy by average expansion order in continuous time – hybridization expansion Monte Carlo simulations

$$\epsilon_K = -k_B T < k >$$

Haule, K., 2007, Phys. Rev. B 75, 155113

Results for heterostructure

Average order expansion in Monte Carlo simulation (kinetic energy)



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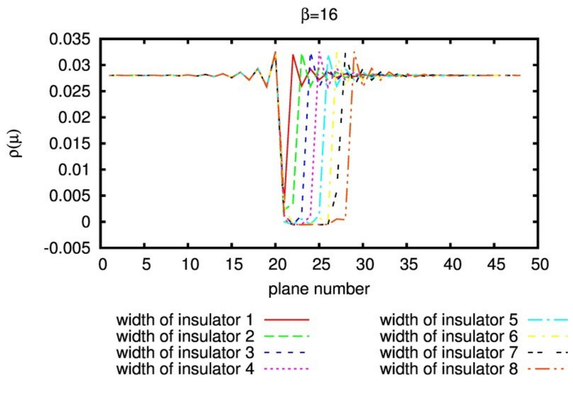

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