Vladimir A Gavrichkov, J Material Sci Eng 2017, 6:4(Suppl)
DOI: 10.4172/2169-0022-C1-067

Microscopic background in metal-insulator criterion for doped Mott-Hubbard materials

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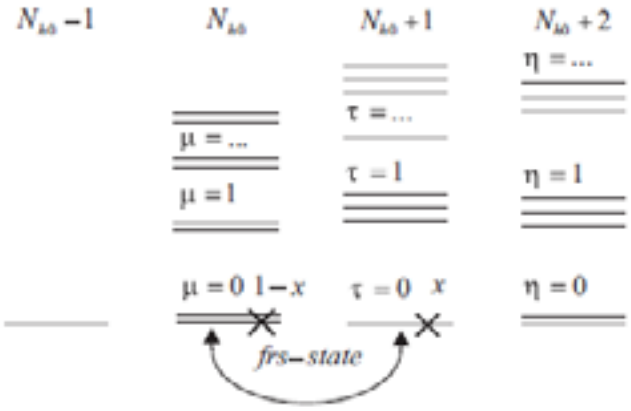
Statement of the Problem: The purpose of this study is to construct a metal–insulator criterion based on Wilson's ideas concerning a system of itinerant electrons in the analytical form for the doped Mott–Hubbard materials and also to associate a microscopic background of criterion with real properties of these materials.

Methodology & Theoretical Orientation: For our purposes, it is convenient to start with Lehmann's representation for the Green's function $G^{\lambda\lambda}_{fg,\sigma} = \left\langle\left\langle c_{f\lambda\sigma} \middle| c^{+}_{g\lambda\sigma} \right\rangle\right\rangle$ of the intra-cell Hamiltonian with respect to the family of single-particle operators $c^{(+)}_{f\lambda\sigma}$ and their matrix elements in the basis of $\left|(N_h, M_S)_i\right\rangle$ eigenstates of $\hat{H}_0$ (S and M are the spin and spin projection of the many-electron cell eigenstate), where index *i* runs over, μ, τ and ή and states in the different sectors of configuration space in Figure from the work.

Findings: By following this approach, one obtains a simple metal– insulator criterion, which is characterized by the condition: the number of first removal electron (*frs*) states $N_{frs} = 0$ (-insulator) or $N_{frs} > 0$ (-metal) irrespective of the doped hole concentration x.

Conclusion & Significance: We suggest a non-adiabatic origin of the forbidden *frs* states and Ham's effect for their matrix elements as the probable reasons for insulator state of the doped materials with translational symmetry.



Biography

Vladimir A Gavrichkov has experience in the study of the electronic structure of strongly correlated materials: iron borates with spin S=5/2, manganites (S=2) and cuprates (S=1/2).

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