Role of inter-site Coulomb interaction on charge and stripe order of La$_{2-x}$Sr$_x$NiO$_4$

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La$_{2-x}$Sr$_x$NiO$_4$ (LSNO) shows novel charge and spin stripe order whose period depends on the value of $x$ and is insulator throughout in the range of $0 \leq x < 0.9$ at low temperatures. [1] There are two candidates for the origin of the stripe order. One is Jahn-Teller mechanism and the other is long ranged Coulomb interaction.

Recently we have studied these systems with $x=0$, 1/3, 1/2, 1 by using LSDA+U method. [2] The results of mother material LSNO ($x=0$) and low-doped LSNO ($x=1/3$) show good agreement with observed width of energy gap and localized spin moment. LSNO of $x=0$ is antiferromagnetic insulator where each Ni ion is Ni$^{2+}$. In the LSNO ($x=1/3$), hole is localized on the $x^2-y^2$ orbital of Ni$^{3+}$ site. In the result of LSNO ($x=1$) by using LSDA+U method, hole is doped into $3z^2-1$ orbitals of Ni ions due to the strong on-site Coulomb interaction in contrast to hole in LSNO ($x=1/3$). In real LSNO ($x=1/2$), hole is doped into $3z^2-1$ orbital. The LSDA+U result, however, becomes an unrealistic antiferromagnetic metal. A real ground state should be paramagnetic metal and its wavefunction a linear combination of Slater determinants with different spin configurations. In the result of LSNO ($x=1/2$) by using LSDA+U, hole is not localized on specific site. Consequently, the system is metal. The real LSNO ($x=1/2$) shows charge and spin stripe order and is insulator. It is more puzzling than the case of LSNO ($x=1$), because the wavefunction of band insulator is well described with a single Slater determinant.

In the LSNO, two $e_g$ orbitals of Ni ion are relevant. We constructed double orbital extended Hubbard model Hamiltonian for $x=1/2$ system based on the LDA calculation and solved its exact ground state. On-site Coulomb and exchange interaction parameters $U$ and $J$ are imported from LSDA+U calculation. The ground state changes depending on the value of inter-site Coulomb interaction $V$. The ground state with $0<V<0.41$ does not show charge order while $0.41<V<1$ does. We chose the value $V=0.5$eV, which is consistent with that of 0.34eV in RPA calculation of LaMnO$_3$. [3] Charge and spin order are discussed by using charge-charge and spin-spin correlation function respectively. And the transport property is discussed by using single particle spectral function.

Analytic continuation of the ground state wavefunction at $V=0.5$eV to $V=0$eV causes degenerated single electron state at Fermi level. Thus the inter-site Coulomb interaction stabilizes charge order and causes energy gap opening at Fermi energy. Spin order in real LSNO ($x=1/2$) is understood by introducing anisotropy of second nearest neighbor hopping integrals, which is different from usual Jahn-Teller mechanism, into the model Hamiltonian. The LSDA+U result does not shows charge order, since it does not include the correlation effect induced by $V$, such as self-interaction of Ni$^{2+}$ $x^2-y^2$ orbital with its tail on Ni$^{3+}$ site.