MAGNETIC POLARON IN MAGNETIC PEROVSKITES

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Abstract. We study magnetic polaron (MP): electron trapped in ferromagnetic droplet, which is surrounded by antiferromagnetic media in one dimensional case and classical t2g spin approximation. It is shown that the ground state energy of MP is unstable towards the Coulomb electron - electron repulsion. The size of MP corresponding to the size of ferromagnetic droplet is also studied numerically. A possibility to apply this model for explaining of magnetic phase separation in magnetic perovskites is discussed.

The nano-scale phase separation and Colossal Magnetoresistance (CMR) effect are studied intensively both in theoretical and experimental aspects (see [1]). Nagaev practically proposed the idea of inhomogeneous state and phase separation in magnetic semiconductors much earlier [2]. The compounds, which appear to form "nanoscale phase separation", have at least two competing phases. These phases with specific types interactions reach a compromise by forming inhomogeneous patterns. These patterns have nano (10-9m) characteristic length scale. In manganites the two competing phases are ferromagnetic (FM) and antiferromagnetic (AF) one. In manganites $Ln_{1-x}A_xMnO_3$ (Ln: rare earth ions; A: Ca, Ba,..), eg electrons of Mn^{+3} are localized in conducting FM droplets, which are distributed inside an AF insulating background. This bound state of electrons is called magnetic polaron (MP). Pathak and Satpathy [3] found an exact solution of continuum model in one dimension for self-trapped MP without an electrons Coulomb repulsion. In this contribution we try to include the Coulomb repulsion in calculation and study the size of. The Hamiltonian of system is written as follows (see [4]):

$$H = -t\sum_{\langle ij\rangle,\sigma} a^{+}_{i\sigma}a_{j\sigma} + HC - J_H\sum_i \vec{s}_i\vec{S}_i + V_0\sum_{\langle i,j\rangle} n_i n_j + J\sum_{\langle i,j\rangle}\vec{S}_i\vec{S}_j \,, \qquad (1)$$

where $a^{+}_{i\sigma}$ ($a_{j\sigma}$) is the creation (annihilation) operator of electron having spin projection σ at i-site. <ij> denotes summation over nearest-neighbor (n. n.) sites. JH is the strong intrasite Hund exchange interaction between electrons eg spin $\vec{s}$ and localized core t2g spin $\vec{S}_i$. V_0 is Coulomb interaction between the n. n. sites electrons. J is AF exchange interaction between t2g spins. The localized spins are treated classically and written in the spherical coordinate system as $\vec{S}_i \equiv S(\sin\theta_i\cos\varphi_i, \sin\theta_i\sin\varphi_i, \cos\theta_i)$. Using unitary transformation Ri to new fermions operators $d^{+}_{i\sigma}$, $d_{i\sigma}$, $a_{i\sigma} = R_{i\sigma\sigma'}d_{i\sigma'}$ and condition of strong coupling limit $J_H \to \infty$ one has " double exchange hamiltonian":

$$H = -\sum_{\langle ij\rangle}\tilde{t}_{ij}c^{+}_i c_j + HC - J_H S\sum_i c^{+}_i c_i + V_0\sum_{\langle i,j\rangle} n_i n_j + JS^2\sum_{\langle i,j\rangle}\cos\chi_{ij} \,, \qquad (2)$$

where $c_i^+(c_i)$ is new creation (annihilation) spinless fermion operator corresponding "spin up" creation $(d_{i\uparrow}^+)$, annihilation $(d_{i\uparrow})$ one. $\tilde{t}_{ij} = t\cos(\chi_{ij}/2)$ is Anderson-Hasegawa electron hopping amplitude. $\chi_{ij} = \theta_i - \theta_j$ is angle between n. n. core spins. The total energy of system in one-dimensional and continuum limit case (see also [4]) is:

$$E = -t\int_{-\infty}^{+\infty}\left\{2\psi^2(x)+\psi(x)\frac{\partial^2\psi(x)}{\partial x^2}\right\}\cos\frac{\chi(x)}{2}dx$$
$$+V_0\int_{-\infty}^{+\infty}\psi^2(x)\left\{\psi^2(x)+\psi(x)\frac{\partial^2\psi(x)}{\partial x^2}+\left(\frac{\partial\psi(x)}{\partial x}\right)^2\right\}dx + JS^2\int_{-\infty}^{+\infty}(\cos\chi(x)+1)dx \tag{3}$$

Following to [3], we choose variational wave function for MP with variation parameter λ and normalized in the one-dimensional space:

$$\psi(x) = \sqrt{\frac{\lambda}{2}}\frac{1}{ch(\lambda x)}. \tag{4}$$

The angle between localized spin vectors depends on second variation parameter η and has chosen as:

$$\chi(x) = 2\arccos\left[\frac{\eta\alpha}{4}\psi^2(x)\right] \text{ if } \frac{\eta\alpha}{4}\psi^2(x) \le 1; \quad \chi(x) = 0 \text{ otherwise.} \tag{5}$$

Here $\alpha = t/(JS^2)$ and crystal lattice constant is taken as a = 1. The ground state energy of system is obtained by minimizing total energy functional over parameters λ, η. The radius of magnetic polaron is given by:

$$\langle x^2\rangle^{1/2} = \int_{-\infty}^{+\infty}\psi^2(x)x^2dx. \tag{6}$$

In the numerical calculation one has to find the minimum value of total energy (3) and corresponding parameter λ, η. With founded λ, η we can estimate the size of polaron according to (6). The numerical calculation for ground state energy and size of MP as function of α parameter for V_0 = 0.2 is given in Table 1 (all types of energy is measured in unit of hopping integral t).

Table 1: Ground state energy of MP as a function of parameter α, V_0 = 0.2. The parameters λ, η were chosen from minimum condition for energy.

V_0	α	E	λ	η	$\langle x^2\rangle^{1/2}$
0.2	1	-0.0592	0.6368	1.7567	0.8034
	2	-0.1438	0.7306	1.6797	0.6537
	5	-0.4037	0.7839	1.6312	0.5882
	10	-0.8387	0.8006	1.6155	0.5699
	20	-1.1722	0.7708	2.9505	0.6033
	30	-1.3473	0.6853	2.7555	0.7196

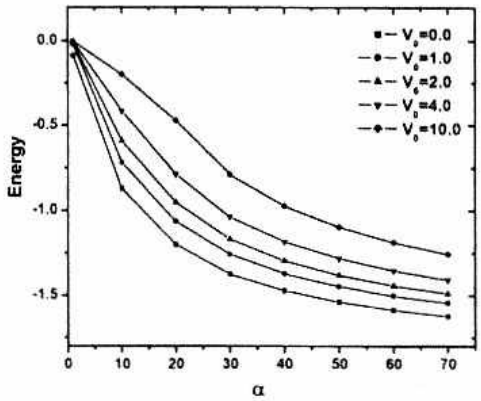

Fig.1. Ground state energy as a function of $\alpha=t/JS^2$ for several V_0 values.

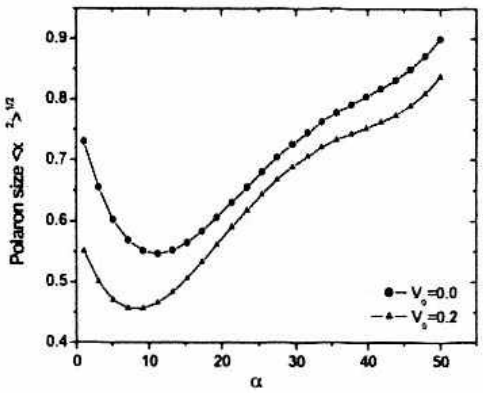

Fig.2. The radius of MP as a function of α for small Coulomb interaction V_0.

Figure 1 shows the α dependence of E for other V_0 values. The radius of MP as function of parameters α, V_0 is also shown in Fig. 2 and Fig.3. According to Fig. 2, the MP radius has minimum for low values of the Coulomb repulsion $V_0<1$ ($V_0<t$ in real energy unit). In other words, V_0 should be smaller than kinetic energy. For large value of V_0 (comparable or larger than kinetic energy) radius of MP may be very large for $\alpha<10$ and small for $\alpha>10$ (Fig. 3). The typical values of parameters of theory for perovskites are: J~0.003 eV, t~0.2 eV, S = 3/2 or α~30. The radius of MP when V_0 = t is order of lattice constant (a ~ 40 nm), then the size of FM droplet is about 80 nm. We have the nanoscale FM droplets embedded in the AF background. This estimation serves good interpretation for the observed experimentally phase separation in manganites.

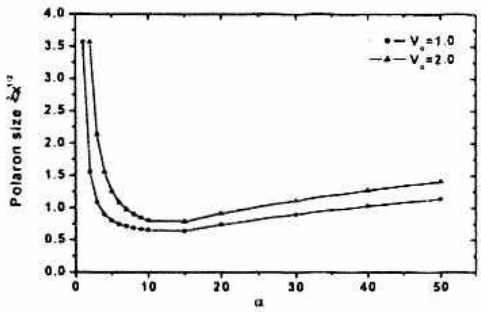

Fig.3. The radius of polaron as a function of α for large values of V_0. The minimum is disappeared for very large V_0.

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