Considerations on the quantum double-exchange Hamiltonian

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Abstract

- Introduced by Zener [1] the notion of double exchange (DE) attracted renewed attention in connection with the colossal magnetoresistive (CMR) effect [2] in mixed-valence manganites (e.g. $La_{1-x}Ca_xMnO_3$).
- Large Coulomb and Hund's rule interaction of manganese d shell electrons, which split into e_g and t_{2g} subbands due to octahedral symmetry, yields a hopping amplitude of the itinerant e_g electrons, that depends on the background of local spins $S = 3/2$ formed by the t_{2g} electrons [3].
- We consider different possibilities for an approximate treatment of the lattice DE Hamiltonian in terms of effective electronic models, which are used in a more elaborate modelling of CMR materials (see our related poster and Ref. [4]).
- Since quantum double exchange on a lattice is most suitably described with the help of Schwinger bosons [5], we review its derivation in terms of Schwinger bosons, consider the semiclassical limit ($S \to \infty$), and, by means of numerical experiments, illustrate how this limit evolves from the quantum case.

Schwinger bosons & double exchange

As a starting point we take the Kondo lattice model including on-site Coulomb repulsion,

$$H = -t \sum_{\langle ij\rangle\sigma} \left[c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}\right] - J_H \sum_{i\sigma\sigma'} (\mathbf{S}_i \boldsymbol{\sigma}_{\sigma\sigma'}) c_{i\sigma}^\dagger c_{i\sigma'} + U \sum_i n_{i\downarrow} n_{i\uparrow}\,. \quad (1)$$

Here summation is over nearest neighbour bonds $\langle ij\rangle$ or sites i, respectively, and $c_{i\sigma}^{(\dagger)}$ denote electrons in a single band, interacting with localized spins S_i via Hund's coupling J_H. For clarity and since it can be included easily in the final result, the orbital degeneracy of the e_g electrons is neglected.

In the manganites we have $U \gg J_H > t$ (cf. Refs. [3, 6]). Hence, we first take the limit $U \to \infty$, resulting in

$$H = -t \sum_{\langle ij\rangle\sigma} \left[\tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + \text{H.c.}\right] - J_H \sum_{i\sigma\sigma'} (\mathbf{S}_i \boldsymbol{\sigma}_{\sigma\sigma'}) \tilde{c}_{i\sigma}^\dagger \tilde{c}_{i\sigma'} \quad (2)$$

with restricted fermions $\tilde{c}_{i\sigma} = c_{i\sigma}(1 - n_{i\,-\sigma})$.

Next, the exchange term is solved and hopping is considered as a small perturbation [7]. Introducing operators, which project locally onto the high-spin state,

$$(P_i^+)_{\sigma\sigma'} = \frac{(\mathbf{S}_i \boldsymbol{\sigma}_{\sigma\sigma'}) + (S+1)\delta_{\sigma\sigma'}}{2S+1}\,, \quad (3)$$

the DE-Hamiltonian is given by (Eq. (2.3), Ref. [7])

$$H_{\text{el}}^{\text{DE}} = -t \sum_{\langle ij\rangle\sigma\sigma'} \left[\tilde{c}_{i\sigma}^\dagger (P_i^+ P_j^+)_{\sigma\sigma'} \tilde{c}_{j\sigma'} + \text{H.c.}\right]\,. \quad (4)$$

This expression can be simplified noticeable with the help of Schwinger bosons a_i and b_i, allowing to describe spins of arbitrary length,

$$S_i^+ = a_i^\dagger b_i\,,\; S_i^- = b_i^\dagger a_i\,, \quad (5)$$

$$S_i^z = (a_i^\dagger a_i - b_i^\dagger b_i)/2\,, \quad (6)$$

$$|S_i| = (a_i^\dagger a_i + b_i^\dagger b_i)/2\,. \quad (7)$$

The projection operators P_i^+ admit of a decomposition,

$$(P_i^+)_{\sigma\sigma'} = \frac{1}{2S+1}\begin{bmatrix} (S+1)+S_i^z & S_i^- \\ S_i^+ & (S+1)-S_i^z \end{bmatrix} = \frac{1}{2S+1}\begin{bmatrix} a_i \\ b_i \end{bmatrix} \cdot \begin{bmatrix} a_i^\dagger & b_i^\dagger \end{bmatrix}\,, \quad (8)$$

which leads to

$$H_{\text{el}}^{\text{DE}} = \frac{-t}{2S+1} \sum_{\langle ij\rangle} \left[(R_i^+)^\dagger (a_i^\dagger a_j + b_i^\dagger b_j) R_j^+ + \text{H.c.}\right] \quad (9)$$

with the projector

$$R_i^+ = \frac{\tilde{c}_{i\uparrow} a_i^\dagger + \tilde{c}_{i\downarrow} b_i^\dagger}{\sqrt{2S+1}}\,. \quad (10)$$

This projector annihilates the electron and transformes the coupled high-spin state into its corresponding Schwinger boson representation, i.e., the electronic spin is absorbed into the boson description.

Hence, it is permitted to replace R_i^+ by spinless fermions c_i, yielding the DE-Hamiltonian in its most compact form,

$$H_{\text{el}}^{\text{DE}} = \frac{-t}{2S+1} \sum_{\langle ij\rangle} \left[(a_i^\dagger a_j + b_i^\dagger b_j) c_i^\dagger c_j + \text{H.c.}\right]\,, \quad (11)$$

with the constraint

$$a_i^\dagger a_i + b_i^\dagger b_i = 2S + c_i^\dagger c_i\,. \quad (12)$$

In the case of low doping usually it is more appropriate and natural to consider holes instead of electrons. Using restricted hole operators $\tilde{h}_{i\sigma}$, Eq. (9) is given by

$$H_{\text{hole}}^{\text{DE}} = \frac{t}{2\bar{S}} \sum_{\langle ij\rangle} \left[(R_i^-)^\dagger (a_i a_j^\dagger + b_i b_j^\dagger) R_j^- + \text{H.c.}\right]\,, \quad (13)$$

with modified projectors,

$$R_i^- = \frac{\tilde{h}_{i\uparrow} b_i - \tilde{h}_{i\downarrow} a_i}{\sqrt{2\bar{S}+1}}\,, \quad (14)$$

and $\bar{S} = S + 1/2$ as a shortcut.

The Hamiltonian for spinless fermions, Eq. (11), changes only little,

$$H_{\text{hole}}^{\text{DE}} = \frac{t}{2\bar{S}} \sum_{\langle ij\rangle} \left[(a_i a_j^\dagger + b_i b_j^\dagger) h_i^\dagger h_j + \text{H.c.}\right] \quad (15)$$

with the constraint

$$a_i^\dagger a_i + b_i^\dagger b_i = 2\bar{S} - h_i^\dagger h_i\,. \quad (16)$$

Note, that on a lattice it is not possible to express this Hamiltonian in terms of permutation and spin operators, e.g. in the form [8]

$$H = -t \sum_{\langle ij\rangle} P_{ij} Q_{\bar{S}}\left(\frac{\mathbf{S}_i \mathbf{S}_j}{\bar{S}(\bar{S}-1/2)}\right)\,, \quad (17)$$

where P_{ij} is a permutaion of neighbouring spin states and $Q_{\bar{S}}(\ldots)$ a polynomial of order $2\bar{S} - 1$.

Effective transport Hamiltonian

To obtain an effective Hamiltonian for the spin-dependent hole-hopping, the spin part of the DE interaction is considered within mean field approximation. However, there are two representations of the DE Hamiltonian to start from: Eqs. (13) and (15). The resulting effective Hamiltonians describe carriers with or without spin, respectively.

Given Eq. (13), a mean hopping of the spin-$\frac{1}{2}$ carriers is obtained averaging $H_{\text{hole}}^{\text{DE}}$ over free spins $\bar{S}$ in a homogeneous field $\lambda = \beta g \mu_B H_{\text{eff}}^z$. Using Eqs. (5)-(6) together with $\langle S^\pm\rangle = 0$ and $\langle S^z\rangle = \bar{S} B_{\bar{S}}[\bar{S}\lambda]$ (with the Brillouin function $B_{\bar{S}}[z]$), we find

$$H_{\text{hole}}^{\text{eff,II}} = \sum_{\langle ij\rangle} \left[\tilde{t}_\uparrow \tilde{h}_{i\uparrow}^\dagger \tilde{h}_{j\uparrow} + \tilde{t}_\downarrow \tilde{h}_{i\downarrow}^\dagger \tilde{h}_{j\downarrow} + \text{H.c.}\right] \quad (18)$$

with

$$\tilde{t}_\uparrow = \frac{t}{(2\bar{S})(2\bar{S}+1)}\left[\bar{S}(1 - B_{\bar{S}}[\bar{S}\lambda])\right]^2\,, \quad (19)$$

$$\tilde{t}_\downarrow = \frac{t}{(2\bar{S})(2\bar{S}+1)}\left[\bar{S}(1 + B_{\bar{S}}[\bar{S}\lambda])\right]^2\,. \quad (20)$$

In a highly polarized background ($\lambda \to \infty$) the spin-up band can be neglected, whereas in general, the situation is complicated by the fact that Eq. (18) involves restricted fermion operators (Hubbard operators).

Alternatively, an effective Hamiltonian involving spinless carriers is obtained from Eq. (15) by considering a single bond $\langle ij\rangle$ within the ordering field λ, cf. Ref. [7]. The total bond spin S_T yields the matrix element [3]

$$\frac{a_j^\dagger a_i + b_j^\dagger b_i}{2\bar{S}} |S_T, S_T^z\rangle_{(\bar{S}\bar{S})} = \frac{S_T + \frac{1}{2}}{2\bar{S}} |S_T, S_T^z\rangle_{(\bar{S}\bar{S})}\,. \quad (21)$$

Averaged over all values of S_T and S_T^z the corresponding effective Hamiltonian reads

$$H_{\text{hole}}^{\text{eff,I}} = \tilde{t}^{(b)} \sum_{\langle ij\rangle} \left[h_i^\dagger h_j + \text{H.c.}\right]\,, \quad (22)$$

with $\tilde{t}^{(b)} = \gamma_{\bar{S}}[\bar{S}\lambda]\, t$ and

$$\gamma_{\bar{S}}[\bar{S}\lambda] = \tfrac{1}{2} + \tfrac{\bar{S}}{2\bar{S}+1}\coth\left(\tfrac{2\bar{S}+1}{2}\lambda\right)\left[\coth(\bar{S}\lambda) - \tfrac{1}{2\bar{S}}\coth\left(\tfrac{\lambda}{2}\right)\right]\,. \quad (23)$$

Below we compare the classical limit of both, this Hamiltonian and the exact expression.

Classical limit of the DE model

The limit $S \to \infty$ of $H_{\text{el}}^{\text{DE}}$, Eq. (11), is easily derived by taking its expectation value with spin coherent states [10],

$$|\Omega(S,\theta,\phi)\rangle = \frac{(ua^\dagger + vb^\dagger)^{2S}}{\sqrt{(2S)!}}|0\rangle\,, \quad (24)$$

where $u = \cos(\theta/2)e^{i\phi/2}$ and $v = \sin(\theta/2)e^{-i\phi/2}$. Using the properties of coherent states,

$$a\,|\Omega(S,\theta,\phi)\rangle = \sqrt{2S}\;u\;|\Omega(S - \tfrac{1}{2},\theta,\phi)\rangle \quad (25)$$

$$b\,|\Omega(S,\theta,\phi)\rangle = \sqrt{2S}\;v\;|\Omega(S - \tfrac{1}{2},\theta,\phi)\rangle\,, \quad (26)$$

for a given spin configuration $\{\theta_k, \phi_k\}$ and two electronic states $|\psi_1\rangle$ and $|\psi_2\rangle$,

$$|\psi_j\rangle = \prod_k |n_{j,k}\rangle |\Omega(S + \tfrac{n_{j,k}}{2}, \theta_k, \phi_k)\rangle \quad (27)$$

(where $|n_{j,k}\rangle = (c_k^\dagger)^{n_{j,k}}|0\rangle$ with numbers $n_{j,k} \in \{0,1\}$), we find the average

$$\langle\psi_1|H_{\text{el}}^{\text{DE}}|\psi_2\rangle = \prod_k \langle n_{1,k}| \Big(-\sum_{\langle ij\rangle}\left[t_{ij} c_i^\dagger c_j + \text{H.c.}\right] \Big) \prod_k |n_{2,k}\rangle \quad (28)$$

with the matrix element

$$t_{ij} = \cos\left(\frac{\theta_i}{2}\right)\cos\left(\frac{\theta_j}{2}\right)e^{-i(\phi_i - \phi_j)/2} + \sin\left(\frac{\theta_i}{2}\right)\sin\left(\frac{\theta_j}{2}\right)e^{i(\phi_i - \phi_j)/2}\,. \quad (29)$$

Hence, the classical Hamiltonian should read

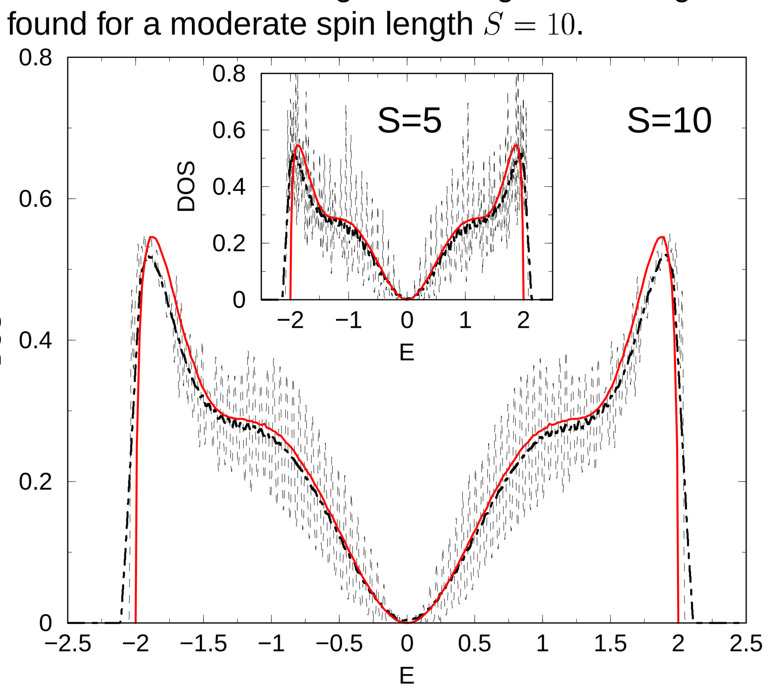
$$H_{\text{class}}^{\text{DE}} = -\sum_{\langle ij\rangle} \left[t_{ij} c_i^\dagger c_j + \text{H.c.}\right]\,, \quad (30)$$

which is equivalent to the results obtained in Refs. [9, 8].

Numerical experiments

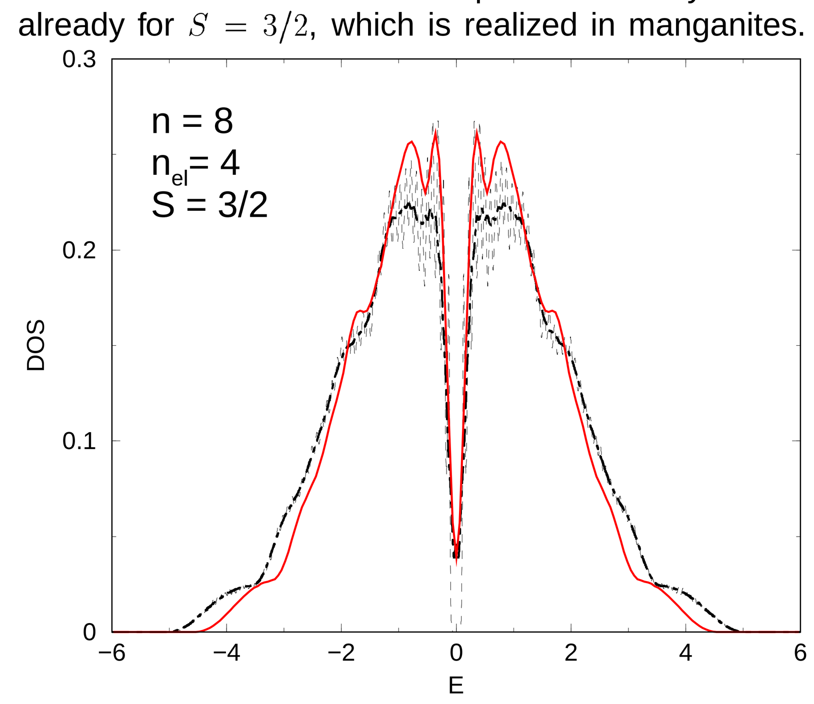
To check the quality of the semiclassical approximation we compare the (canonical) density of states (DOS) for a fixed number of carriers on a small cluster, which interact with quantum (Eq. (11)) or classical (Eq. (30)) spins, respectively.

- Using Chebychev expansion and maximum entropy methods [11], for the quantum case the spectra can be obtained numerically for rather large S. The classical DOS is found by averaging the eigenvalues of $H_{\text{class}}^{\text{DE}}$, Eq. (30), over a large number of spin configurations.
- For two electrons on a ring of 4 sites good convergence is found for a moderate spin length $S = 10$.



Here the black dot-dashed line denotes the running average over the discrete spectrum (thin dashed), whereas the classical limit is given in red.

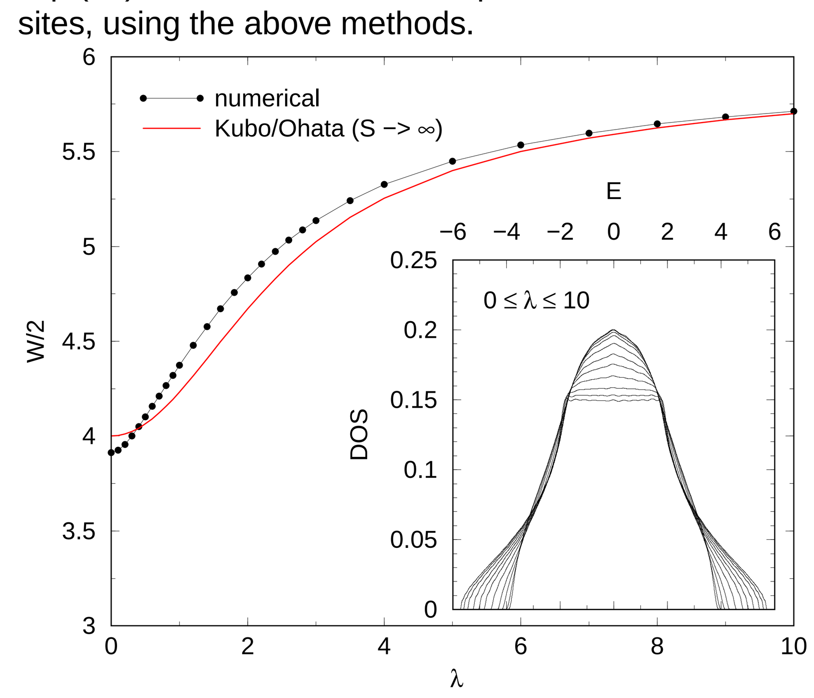
- For 4 electrons and 8 sites the spectra look very similar already for $S = 3/2$, which is realized in manganites.



- Note, that in both figures we subtracted the peak at $E = 0$ consuming a large fraction of spectral weight.

Another interesting check concerns the semi-classical limit of the effective model, Eq. (22).

- The grand-canonical DOS of the tight-binding model, Eq. (30), is calculated for a simple cubic cluster of 64^3 sites, using the above methods.



- Comparing the resulting bandwidth with the limit $S \to \infty$ of $\tilde{t}^{(b)} = \gamma_{\bar{S}}[\bar{S}\lambda]\, t$,

$$\gamma_{\bar{S}\to\infty}[\lambda] = \frac{1}{2}\left(1 + \coth(\lambda)\left[\coth(\lambda) - \frac{1}{\lambda}\right]\right)\,, \quad (31)$$

rather satisfactory agreement is found.

Conclusions

- We review the subject of double exchange using Schwinger bosons and derive an effective Hamiltonian for the spin-dependent hopping of holes in an averaged background of local spins.
- In a related work these results are used within a two-phase scenario for the description of colossal magnetoresistant manganites.

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References

[1] C. Zener, Phys. Rev. **82**, 403 (1951).

[2] S. Jin, T. H. Tiefel, M. McCormack, R. A. Fastnach, R. Ramesh, and L. H. Chen, Science **264**, 413 (1994).

[3] P. W. Anderson and H. Hasegawa, Phys. Rev. **100**, 675 (1955).

[4] A. Weiße, J. Loos, and H. Fehske, arXiv:cond-mat/0101235 (2001).

[5] S. K. Sarker, J. Phys. Condens. Matter **8**, L515 (1996); D. P. Arovas and F. Guinea, Phys. Rev. B **58**, 9150 (1998); S. Ishizaka and S. Ishihara, Phys. Rev. B **59**, 8375 (1999); R. Kilian, PhD thesis, Technische Universität Dresden, (1999); K. Penc and R. Lacaze, Europhys. Lett. **48**, 561 (1999); R. Y. Gu, Z. D. Wang, S.-Q. Shen, and D. Y. Xing, Phys. Rev. B **61**, 1211 (2000).

[6] A. E. Bocquet, T. Mizokawa, T. Saitoh, H. Namatame, and A. Fujimori, Phys. Rev. B **46**, 3771 (1992); J. Zaanen and G. A. Sawatzky, J. Solid State Chem. **88**, 8 (1990); T. Mizokawa and A. Fujimori, Phys. Rev. B **51**, 12880 (1995).

[7] K. Kubo and N. Ohata, J. Phys. Soc. Jpn. **33**, 21 (1972).

[8] E. Müller-Hartmann and E. Dagotto, Phys. Rev. B **54**, R6819 (1996).

[9] E. M. Kogan and M. I. Auslender, Phys. Status Solidi B **147**, 613 (1988).

[10] A. Auerbach, *Interacting Electrons and Quantum Magnetism*, Springer-Verlag, (New York 1994).

[11] R. N. Silver, H. Röder, A. F. Voter, and J. D. Kress, J. Comp. Phys. **124**, 115 (1996); R. N. Silver and H. Röder, Phys. Rev. E **56**, 4822 (1997); B. Bäuml, G. Wellein, and H. Fehske, Phys. Rev. B **58**, 3663 (1998).