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Effective Charge-Spin Models for the Low Energy Excitations in Quantum Dots

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It is shown that the few, strongly correlated electrons in quantum dots can be described by a lattice model at low energies which for many dot-geometries reduces to a spin model. This can be achieved since the low electron density localizes the electrons near their classical ground-state positions. Some cases require a generalization of the Heisenberg model to include 'ring' processes, which involve cyclic rotations of more than two electrons. The energy spectra from these effective models are compared with exact and other approximative results.

Electrical [1] and optical [2] properties of extremely small semiconducting nanostructures depend on the discrete excitation energies and on the spin [3] of the electron system. Such 'quantum dots' have been referred to as 'artificial atoms' [4] since the number N of conducting electrons can be smaller than ten or twenty. Correlations are extremely important when the effective density is low and the electrons are confined to one or two dimensions in the dot [5], restricting calculations to very small N. The (pre-) crystallized charge density distributions for the electrons [6] motivated the approximation within many body pocket states [7] at low energies. The results obtained agree well with numerical solutions for $N \leq 4$.

Here we shall demonstrate that the low energy excitations can be represented by spin models, enabling larger systems to be dealt with and providing new insight into their behaviour. In contrast to magnetic insulators, the atomic lattice constant loses its significance at much larger Fermi wave lengths. The mapping to an effective charge-spin model has been justified by starting with approximate pocket states which are direct products of non-orthogonal one-electron wavefunctions localized near their classical ground state positions, determined by electrostatics [8]. Orthogonalizing these one-electron orbitals and forming all possible antisymmetrized products including spin (Slater determinants), gives a restricted basis set for the problem. Within this restricted basis set, the Hamiltonian is equivalent to a single-band Hubbard model augmented with a direct exchange term and further hopping and Coulomb terms than usually considered. High-energy base-states in which two electrons occupy the same orbital may be eliminated by degenerate perturbation theory resulting, finally, in an effective charge-spin Hamiltonian for the low energy physics [9],

$$H_{\rm eff}^{tJV} = P\sum_{ij}\Big[\sum_{\sigma}(t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+{\rm hc})+ J_{ij}(\boldsymbol{s}_i\cdot\boldsymbol{s}_j-1/4)n_in_j+V_{ij}n_in_j\Big]P \qquad (1)$$

where P projects out states containing doubly occupied 'sites', t_{ij} is an effective hopping from occupied to unoccupied sites and V_{ij} is an effective Coulomb interaction between singly occupied sites. The effective exchange interaction, $J_{ij} = \frac{4|t_{ij}|^2}{U_i - V_{ij}} - j_{ij}$ (with U_i the Hubbard on-site Coulomb matrix element), consists of a superexchange contribution (first term) which favours antiferromagnetic coupling and is usually larger than the direct exchange contribution, j_{ij}.

The low energy spectra calculated from (1) agree exactly with the spectra and spin values obtained by the pocket state method for square well systems in 1D and in 2D as they were investigated in [7]. They also agree well with available exact numerical results ($N \leq 4$ in a hard wall box in 1D and $N = 2$ in the hard wall square [10]). Often the number of electrons equals the number of lattice points when (1) reduces to an antiferromagnetic Heisenberg model.

In some geometries, ring exchange processes can

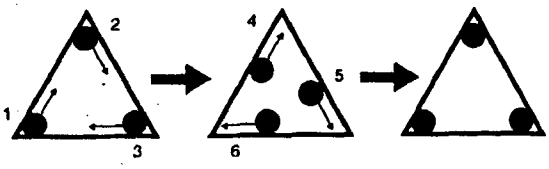

Figure 1: Lattice points for the triangular quantum dot. In the ground manifold all three electrons will be close to the corners. States corresponding to occupation of the intermediate 'sites' are higher in energy by V. The arrows indicate a six-step ring process for the three electrons.

become comparable with, and even exceed, two electron exchange processes. A simple example is a triangular dot in 2D with $N = 3$. The antiferromagnetic Heisenberg model will yield a ground state with total spin $S = 1/2$. However, the triangle can easily be distorted so that now the amplitude for cyclic exchanges of the three electrons is larger than the pair exchanges. This results in a spin polarized $S = 3/2$ ground state. In the usual lattice models these processes correspond to high orders in t/U and are therefore negligible at low densities. However, this is clearly not necessarily the case for the *continuous* electron problem since the electrons can move to intermediate positions with little cost in energy. This is demonstrated by the pocket state approach for which the relative importance of ring contributions as compared to the pair exchange rate can be estimated by the multidimensional WKB approximation. We can model these ring processes in our lattice model by introducing intermediate lattice points which are unoccupied in the ground manifold. This is indicated schematically in Figure 1 for the triangle. The amplitude for a cyclic exchange of the three electrons $\propto t^6/V^5$ and this can be larger than the pair exchange, $\sim 4t^2/U$ in second order since $V \ll U$ (see also [11]). When the Heisenberg model is augmented with the ring processes described above we again get perfect agreement with spectra obtained from the pocket state approximation. Similarly, for larger systems, ring processes involving more than three electrons can be accounted for by introducing suitable intermediate lattice sites.

The effective charge-spin description considerably reduces the computational effort compared to all of the other methods used to date for describing quantum dots. The occurrence of a non-minimal total spin for the ground state in a finite electron system is a direct consequence of the geometry of the boundary (which also includes the influence of a magnetic flux penetrating a ring [12]). In future research this computational advantage together with the new insight that a charge-spin description provides will be investigated systematically and exploited through specific suggestions for experimental design.

REFERENCES

[1] A. T. Johnson *et al.*, Phys. Rev. Lett. **69**, 1592 (1992); J. Weis *et al.*, Phys. Rev. Lett. **71**, 4019 (1993); E. B. Foxman *et al.*, Phys. Rev. B **47**, 10020 (1993).

[2] Ch. Sikorski, U. Merkt, Phys. Rev. Lett. **62**, 2164 (1989); B. Meurer, D. Heitmann, K. Ploog, Phys. Rev. Lett. **68**, 1371 (1992), D. Heitmann, J. P. Kotthaus, in Physics Today, Vol. 56, June (1993).

[3] D. Weinmann, W. Häusler, W. Pfaff, B. Kramer, U. Weiss, Europhys. Lett. **26**, 689 (1994); W. Pfaff, D. Weinmann, W. Häusler, B. Kramer, U. Weiss, Z. Phys. B **96**, 201 (1994); D. Weinmann, W. Häusler, B. Kramer, Phys. Rev. Lett. **74**, 984 (1995).

[4] M. A. Kastner, Rev. Mod. Phys. **64**, 849 (1992).

[5] U. Merkt, J. Huser, M. Wagner, Phys. Rev. B **43**, 7320 (1991); D. Pfannkuche, V. Gudmundsson, P. A. Maksym, Phys. Rev. B **47**, 2244 (1993).

[6] K. Jauregui, W. Häusler, B. Kramer, Europhys. Lett. **24**, 581 (1993).

[7] W. Häusler, Advances in Solid State Physics **34**, 171 (1994); W. Häusler, Z. Phys. B **99**, 551 (1996).

[8] J. H. Jefferson and W. Häusler, preprint (1996).

[9] J. H. Jefferson, J. Phys. C **21**, 1193 (1988); L. F. Feiner, J. H. Jefferson, and R. Raimondi, Phys. Rev. B **51**, 12797 (1995).

[10] G. W. Bryant, Phys. Rev. Lett. **59**, 1140 (1987).

[11] H. Eskes and J. H. Jefferson, Phys. Rev. B **48**, 9788 (1993).

[12] W. Häusler, B. Kramer p. 169 in 'Quantum Dynamics of Submicron Structures', ed. by H. A. Cerdeira, B. Kramer, G. Schön, NATO ASI Series E, Applied Sciences, Vol. 291, Kluwer, Dordrecht (1995); W. Häusler, Physica B (In Press).