# Frustration of antiferromagnetism in the t-t′-Hubbard model at weak coupling

Walter Hofstetter, Dieter Vollhardt

# Frustration of antiferromagnetism in the
# $t$-$t'$-Hubbard model at weak coupling

## W. Hofstetter and D. Vollhardt

Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Universität Augsburg, D-86135 Augsburg, Germany

**Abstract.** The perfect-nesting instability towards antiferromagnetism of the Hubbard model is suppressed by next-nearest neighbor hopping $t'$. The asymptotic behavior of the critical coupling $U_c(t')$ at small $t'$ is calculated in dimensions $d = 2, 3, \infty$ using Hartree theory; this yields the exact result at least in $d > 2$. The order of the transition is also determined. A region of stability of a metallic antiferromagnetic phase in $d = 3$ is identified.

## 1 Introduction

Microscopic investigations of strongly correlated electron systems are usually based on lattice models, the simplest of which is the one-band Hubbard model. In this model two particularly important features of real materials, the structure and the dimension of the underlying lattice, enter only via the kinetic energy. In the past, most model calculations started from a given lattice (mostly hypercubic) and, for simplicity, assumed the hopping to be restricted to nearest neighbors (NN). In this case lattices are either bipartite or not. In dimensions $d > 1$ and at half filling bipartite lattices generically lead to an antiferromagnetic instability in the ground state for any $U > 0$ due to Fermi surface nesting.

It has recently become clear, however, that pure NN-hopping with amplitude $t$ cannot account for some important features of correlated systems and that next-nearest neighbor (NNN) hopping with amplitude $t'$ has to be included for both qualitative and quantitative reasons. Indeed, realistic band structures, photoemission data and neutron-scattering measurements of high-$T_c$ and related materials usually cannot be fit by an energy dispersion that originates solely from NN-hopping [1–4]; estimates for $|t'/t|$ range from 0.15 to 0.5. A particularly clear-cut example is the antiferromagnetic insulator $Sr_2CuO_2Cl_2$ where the inclusion of a $t'$-term is essential to understand the ARPES data [4]. The hole motion in the $t$-$J$ model is also greatly affected by NNN-hopping [5]. Furthermore, it became clear only most recently that the stability of metallic ferromagnetism in the one-band Hubbard model strongly depends on the presence of a $t'$-term in all dimensions $d \geq 1$ [6–11].

On bipartite lattices in $d \geq 2$ the $t'$-term has profound consequences: the frustration introduced by $t'$ suppresses the perfect-nesting instability towards antiferromagnetism at small $U$. Up to now this effect was mainly studied in $d = 2$. Lin and Hirsch [12] calculated magnetic properties within Hartree theory and by exact diagonalization of small systems. Tremblay et al. [1] studied both magnetic and pairing correlations by quantum Monte-Carlo simulations and a two-particle self-consistent approach. Duffy and Moreo [13] investigated the renormalization of $t'$ by the interaction $U$, and presented results [14] suggesting the existence of an itinerant antiferromagnetic ground state at half-filling. Metallic antiferromagnetic phases are known to exist, for example, in $V_{2-x}O_3$ [15] and $NiS_{2-x}Se_x$ [16].

In this paper we wish to obtain analytic insight into the suppression of the antiferromagnetic nesting instability at small $U$ and half filling due to the frustration introduced by $t'$. To this end we solve the $t$-$t'$ Hubbard model

$$\mathcal{H} = -\sum_{\substack{<ij> \\ \sigma}} t \, (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + \sum_{\substack{(ij) \\ \sigma}} t' \, (c_{i\sigma}^\dagger c_{j\sigma} + h.c.)$$

$$+ U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) - \mu \sum_{i\sigma} n_{i\sigma}. \tag{1}$$

within Hartree theory at $T = 0$ and thereby calculate $U_c(t')$, the critical value of $U$ for the onset of antiferromagnetism. For small $t'$ the results for $U_c$ become asymptotically exact [17], at least in dimensions $d > 2$.

We will calculate $U_c(t')$ explicitly in $d = 2, 3, \infty$, both numerically and analytically and will also determine the order of the transition into the antiferromagnetic state.

## 2 Hartree equations

The Hubbard interaction is purely local and therefore does not include any direct exchange. Consequently, there is no Fock term and Hartree-Fock theory reduces to Hartree theory. Within that approach spontaneous symmetry breaking with an antiferromagnetic order parameter (Néel order) is introduced by the ansatz $\langle n_{i\sigma} \rangle = \frac{1}{2}(1 + \sigma(-1)^{|i|}\Delta)$ with $\sigma = \pm 1$, where $\Delta$ is the staggered magnetization. We can then decompose the electron number operator into its expectation value and a fluctuating part $: n_{i\sigma} :$ according to $n_{i\sigma} =: n_{i\sigma} : + \langle n_{i\sigma} \rangle$. Neglecting terms quadratic in the fluctuations, the Hartree Hamiltonian takes the form

$$\mathcal{H}_H = \frac{UN\Delta^2}{4}$$

$$+ \sum_{\substack{\sigma \\ k \in \frac{1}{2}B.Z.}} \left( c_{k\sigma}^\dagger, c_{k+Q\sigma}^\dagger \right) \begin{pmatrix} \varepsilon_k - \mu & -\sigma \frac{U\Delta}{2} \\ -\sigma \frac{U\Delta}{2} & \varepsilon_{k+Q} - \mu \end{pmatrix} \begin{pmatrix} c_{k\sigma} \\ c_{k+Q\sigma} \end{pmatrix}, \tag{2}$$

where the summation is restricted to half of the Brillouin zone. Here we have introduced the number of sites $N$ and the nesting vector $\mathbf{Q} = (\pi, \ldots, \pi)$. The dispersion of the free electrons on the lattice is given by

$$\varepsilon_{\mathbf{k}} = -2t \sum_{i=1}^{d} \cos k_i + 4t' \sum_{i<j}^{d} \cos k_i \cos k_j. \tag{3}$$

For $t' \neq 0$ the perfect nesting property $\varepsilon(\mathbf{k}) = -\varepsilon(\mathbf{k} + \mathbf{Q})$ of the free dispersion no longer holds. In the following we shall use the notation $\mathbf{k}' = \mathbf{k} + \mathbf{Q}$. After diagonalization of the above quadratic form the mean-field Hamiltonian can be written as

$$\mathcal{H}_H = \sum_{\mathbf{k}\sigma} (\tilde{\varepsilon}_{\mathbf{k}} - \mu) \tilde{c}_{\mathbf{k}\sigma}^{\dagger} \tilde{c}_{\mathbf{k}\sigma} + \frac{U N \Delta^2}{4} \tag{4}$$

with the single particle energies

$$\tilde{\varepsilon}_{\mathbf{k}} = \frac{1}{2}\left( \varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k}'} + (\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'})\sqrt{1 + \frac{U^2\Delta^2}{(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'})^2}} \right). \tag{5}$$

Since $\varepsilon_{\mathbf{k}}$ does not fulfill the perfect nesting condition, one has to adjust the chemical potential as a function of $\beta$, $\Delta$, $U$ and $t'$ to ensure the correct filling $n = 1$. In addition, the value of the order parameter $\Delta$ is determined self-consistently by the condition that the free energy

$$F[\beta, \Delta, U] = -\beta^{-1} \ln \operatorname{Tr} \exp(-\beta \mathcal{H}) + \mu N, \tag{6}$$

be minimal with respect to $\Delta$. This leads to two self-consistency equations:

$$1 = \frac{2}{N} \int \frac{d^d k}{(2\pi)^d} f(\beta, \tilde{\varepsilon}_{\mathbf{k}} - \mu) \tag{7}$$

$$1 = \frac{2U}{N} \int \frac{d^d k}{(2\pi)^d} f(\beta, \tilde{\varepsilon}_{\mathbf{k}} - \mu) \frac{1}{(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'})\sqrt{1 + \frac{U^2\Delta^2}{(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'})^2}}}, \tag{8}$$

where $f(\beta, \tilde{\varepsilon}_{\mathbf{k}} - \mu)$ is the Fermi function. The trivial solution $\Delta = 0$ of the minimum condition has been excluded in (8). In the following, (8) and (7) will be analyzed for dimensions $d = 2, 3$ and $\infty$ at $T = 0$.

## 3 Results and discussion

### 3.1 $d = 2$

We set $t = 1$. The presence of $t' \neq 0$ prevents an analytic evaluation of the integrals in (7) and (8). We therefore computed them numerically by k-summation on reciprocal lattices of sizes up to $8000 \times 8000$. Introducing the notation
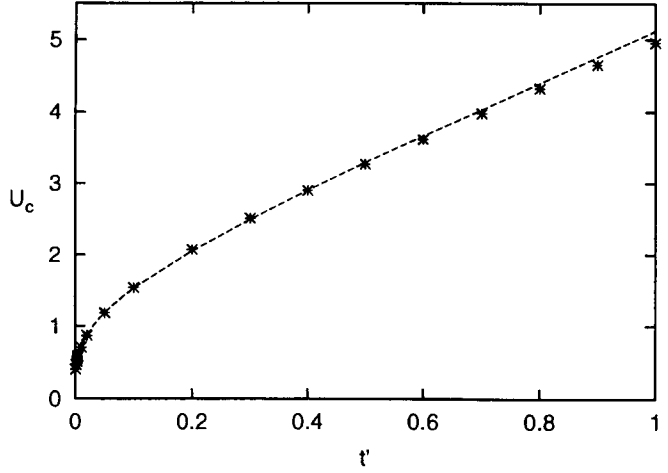
**Fig. 1** Critical interaction $U_c$ vs. next-nearest neighbor hopping matrix element $t'$ in $d = 2$. Dashed line: asymptotic behaviour (11)

$$\gamma := \frac{U\Delta}{2} \tag{9}$$

for the energy gap of the Hartree dispersion (5), we notice that both the integrals in (7) and (8) only depend on $\gamma$.

We find that for any $t' \neq 0$, the integral in (8) has a finite limit for $\gamma \to 0$. This implies that below a critical value $U_c$ of the interaction a stable solution with $\Delta > 0$ no longer exists. For $d = 2$ this fact was already noted by Lin and Hirsch [12]. The dependence of $U_c$ on $t'$ is shown in Fig. 1. For $t' \to 0$, $U_c(t')$ decreases very slowly. An analytic description of the behavior of $U_c(t')$ may be obtained by noting that the divergence of the integral in (8) for $t' = 0$ is cut off just at the value of $\gamma$ where the indirect bandgap [18] in the Hartree dispersion (5) closes, namely at

$$\gamma^* = 2t'. \tag{10}$$

The asymptotic behaviour of $U_c(t')$ for small $t'$ may thus be found by setting $t' = 0$ in (8) and using $\gamma^*$ as a cut-off. This leads to

$$[U_c(t')]^{-1} = c_1 \int_0^4 d\varepsilon \, K\left(\sqrt{1 - \left(\frac{\varepsilon}{4}\right)^2}\right) \frac{1}{\sqrt{\varepsilon^2 + (2t')^2}} \tag{11}$$

where $K$ is the complete elliptic integral and $c_1 = 1/(2\pi^2)$. The approximation (11) is very good up to $t' \approx 1$, as can be seen in Fig. 1. For small $t'$, (11) reduces to [17]

$$[U_c(t')]^{-1} = \frac{c_1}{2} (\ln t')^2 + c_2 \ln t' \tag{12}$$

where $c_2 \approx -0.15$. The quadratic dependence of $U_c$ on $\ln t'$ is characteristic for $d = 2$, where the logarithmic divergence of the density of states (DOS) for $t' = 0$ at the Fermi level introduces an additional factor $\ln t'$.

The behaviour of the order parameter $\Delta$ at $U \approx U_c$ can be characterized as follows: For $t'$ below a threshold value $t'_0 \approx 0.4$ the order parameter $\Delta$ jumps to 0 dis-
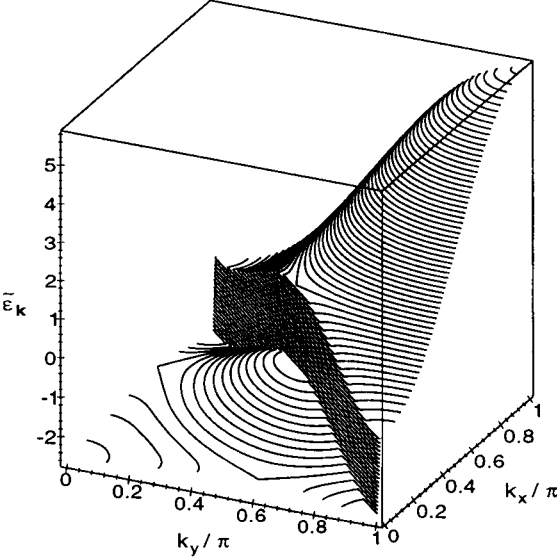
**Fig. 2** Hartree dispersion $\tilde{\varepsilon}_k$ in $d = 2$ for $t' = 0.4$ and $\gamma = 1.0$ with an indirect bandgap between $(\pi/2, \pi/2)$ and $(0, \pi)$

continuously when the interaction is reduced below $U_c(t')$, indicating a first order phase transition. For $U > U_c$, the order parameter takes exactly the same value as for $t' = 0$. For $t' > t'_0$ and $U \to U_c$ the order parameter goes to zero continuously, but extremely fast.

### 3.2 $d = 3$

We evaluate the Hartree equations numerically at zero temperature, using lattice sizes up to $400 \times 400 \times 400$. As before we notice that the divergence of the integral in (8) for $\gamma \to 0$ is cut off for any finite $t'$. The resulting critical interaction $U_c(t')$ is shown in Fig. 3. The indirect bandgap again closes at $\gamma^* = 2t'$, but in this case the order parameter goes to zero continuously as $U \to U_c$, indicating a second-order phase transition. The logarithmic divergence of the integral in (8) is cut off at $\gamma^*$, which leads to the asymptotic expression [17]

$$[U_c(t')]^{-1} = -c_3 \ln t' + c_4, \tag{13}$$

where $c_4 \approx 0.25$ is a fit parameter and $c_3 = N(0) \approx 0.14$, with $N(0)$ as the DOS at the Fermi level in $d = 3$ for $t' = 0$. Eq. (13) represents a good fit for $t' < 0.4$.

### 3.3 $d = \infty$

To analyze the model (1) on a hypercubic lattice in the limit of infinite dimensions, one has to ensure that the hopping remains finite; this is achieved by the scaling [19, 20]
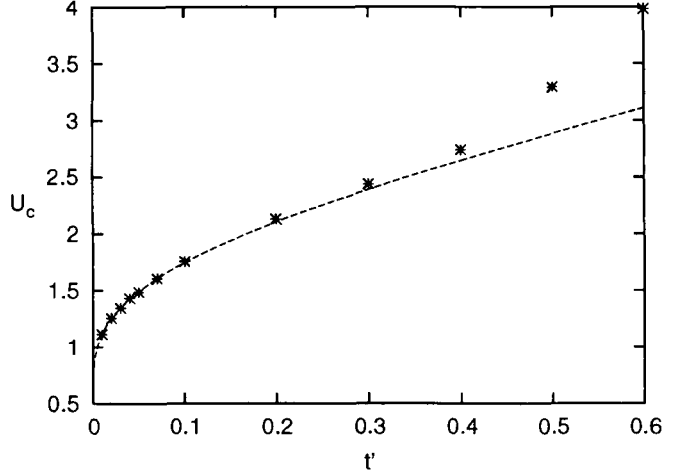
**Fig. 3** Critical interaction $U_c$ vs. $t'$ in $d = 3$. Dashed line: asymptotic behavior (13)

$$t = \frac{t^*}{\sqrt{2d}} \;, \qquad t' = \frac{t'^*}{\sqrt{2d(d-1)}} \tag{14}$$

for the NN- and NNN-terms, respectively. In the following we set $t^* = 1$. As shown by Müller-Hartmann [20] the dispersion of the free electrons then reduces to

$$\varepsilon(\mathbf{k}) \rightarrow \varepsilon - \frac{t'^*}{\sqrt{2}}(1 - \varepsilon^2). \tag{15}$$

Here $\varepsilon$ is the kinetic energy without the $t'^*$-term, which has a Gaussian distribution [19]

$$N(\varepsilon) = \frac{1}{\sqrt{2\pi}} \exp\left(\frac{\varepsilon^2}{2}\right). \tag{16}$$

As a result, we can write the Hartree dispersion in the form

$$\tilde{\varepsilon} = \frac{1}{2}\left\{ +\sqrt{2}\, t'^*\left(\varepsilon^2 - 1\right) + 2\varepsilon\sqrt{1 + \frac{U^2\Delta^2}{4\varepsilon^2}} \right\}; \tag{17}$$

as before, it only depends on $t'^*$ and $\gamma = U\Delta/2$. We note that due to the exponential band-tails of the hypercubic DOS there is no true gap between the two Hartree bands for any value of $\gamma$. The Hartree equations can be written as one-dimensional integrals and are readily solved numerically. Again we find a critical interaction $U_c$ for the stability of long-range antiferromagnetic order at $T = 0$. A plot of $U_c(t'^*)$ is shown in Fig. 4. Due to the absence of a band gap, the asymptotic behavior of $U_c$ for small $t'^*$ is qualitatively different from that in $d = 2, 3$. In the present case, the cut-off for the integral in (8) is provided by a small filling in the upper one of the two Hartree bands (17) which vanishes exponentially for $t' \rightarrow 0$ i.e. $\gamma^* \approx \frac{|t'^*|}{2}\exp(-\frac{1}{(t'^*)^2})$. This leads to an asymptotic behaviour [17] of the form
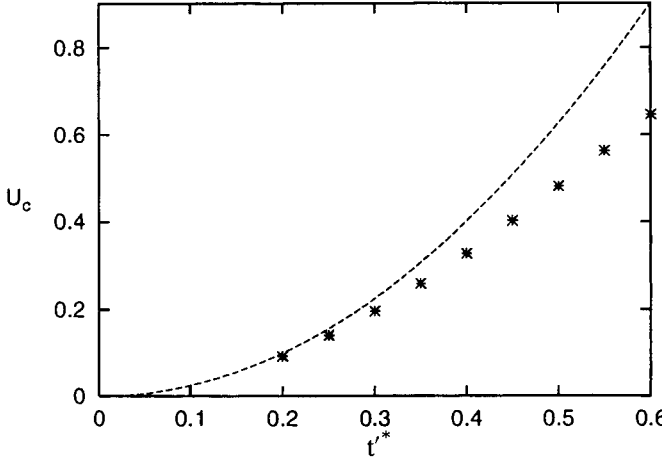
**Fig. 4** Critical interaction vs. $t'^*$ in $d = \infty$. Dashed line: asymptotic behavior (18)
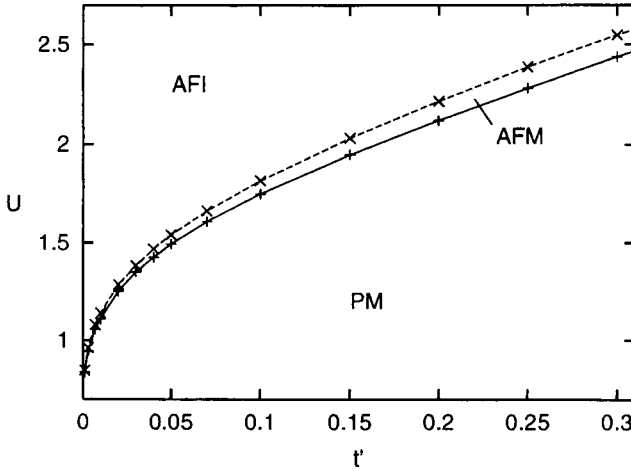


**Fig. 5** Region of stability of a metallic antiferromagnetic phase (AFM) in $d = 3$ in the $U$-$t'$ phase diagram. Full line: $U_c(t')$, dashed line: value of $U$ where the band gap closes. Outside the AFM region the system is either an antiferromagnetic insulator (AFM) or a paramagnetic metal (PM)

$$U_c = c\,(t'^*)^2 \tag{18}$$

where $c \approx \sqrt{2\pi}$. Hence $U_c$ decreases much faster than in $d = 2, 3$. As in $d = 3$ the order parameter $\Delta$ goes to zero continuously for $U \to U_c$. A second-order phase transition is therefore seen to be generic for $d > 2$. We note that, in $d = 3$, the continuously vanishing order parameter implies a (small) range of $U$ values where the band gap is zero but $\Delta$ is still finite. This implies the existence of a *metallic* antiferromagnetic phase for $t' \neq 0$ as shown in Fig. 5. In $d = \infty$, on the other hand, there is never a true bandgap anyway, as described above. Therefore, for $t' \neq 0$ and $U > U_c$, we always find metallic antiferromagnetism. The existence of such a phase was already discussed by Georges et al. [21]. Quite generally, in dimensions $2 \leq d < \infty$ a next-neighbour hopping term $t'$ is found to be very effective in suppressing the perfect nesting instability towards an antiferromagnetic ground state.

## Note added in proof:

In $d = 2$, if the $t'$-hopping occurs only along *one* of the diagonals of the squares, the dispersion reads $\varepsilon_k = -2t\left(\cos k_x + \cos k_y\right) + 2t'\cos(k_x + k_y)$. The corresponding $t - t'$-Hubbard model may be viewed as a simple dimer model of the two-dimensional organic superconductor $\kappa - (\text{BEDT} - \text{TTF})_2 X$ which was investigated by Kino and Fukuyama [J. Phys. Soc. Jpn. **65** (1996) 2158] within Hartree-Fock theory. In contrast to the results of Sect. 3.1, one then obtains a region of stability of an AFM phase which is qualitatively similar to the result for the regular $t - t'$-model in $d = 3$ shown in Fig. 5. The discontinuous transition from the paramagnetic metal into the antiferromagnetic insulator obtained by Kino and Fukuyama is found to occur for $|t'| > 0.6$ when this AFM phase is unstable.

We thank R. McKenzie for drawing our attention to this variant of the $t - t'$-Hubbard model, and to H. Kino and H. Fukuyama for correspondence.

## References

[1] P. Bénard, L. Chen, A.-M.S. Tremblay, Phys. Rev. B **47** (1993) 589; A. Veilleux, A. Daré, L. Chen, Y.M. Vilk, A.-M.S. Tremblay, Phys. Rev. B **52** (1995) 16255
[2] T. Tohyama, S. Maekawa, Phys. Rev. B **49** (1993) 3596
[3] G. Stemmann, C. Pépin, M. Lavagna, Phys. Rev. B **50** (1994) 4075
[4] O.K. Andersen, A.I. Liechtenstein, O. Jepsen, F. Paulsen, J. Phys. Chem. Solids **56** (1995) 1573
[5] A. Schiller, P. Kumar, R. Strack, D. Vollhardt, Phys. Rev. B **51** (1995) 8337
[6] H. Tasaki, Phys. Rev. Lett. **75** (1995) 4678
[7] K. Penc, H. Shiba, F. Mila, T. Tsukagoshi, Phys. Rev. B **54** (1996) 4056
[8] S. Daul, R. Noack, Z. Phys. B **103** (1997) 293
[9] R. Hlubina, S. Sorella, F. Guinea, Phys. Rev. Lett. **78** (1997) 1343
[10] M. Ulmke, Euro. Phys. J. B **1** (1998) 301
[11] J. Wahle, N. Blümer, J. Schlipf, K. Held, D. Vollhardt, cond-mat/9711242
[12] H.Q. Lin, J.E. Hirsch, Phys. Rev. B **35** (1987) 3359
[13] D. Duffy, A. Moreo, Phys. Rev. B**52** (1995) 15607
[14] D. Duffy, A. Moreo, Phys. Rev. B**55** (1997) 676
[15] S. Carter et al., Phys. Rev. Lett. **67** (1991) 3440; W. Bao et al., ibid. **71** (1993) 766
[16] S. Sudo, J. Mag. Mag. Mat. **114** (1992) 57
[17] The Hartree-Fock approximation yields the exact ground state energy for sufficiently small $U$. Nevertheless, weak coupling results for the *ordered* phase of the Hubbard model, e.g. for the order parameter, differ from the corresponding Hartree(-Fock) results by a renormalization factor of order unity [P.G.J. van Dongen, Phys. Rev. Lett. **67** (1991) 757; Phys. Rev. B **50** (1994) 14016]. This implies that the cut-off introduced by $t'$ (see Eqn. (8)) is related to the *exact* cut-off by some factor. Since $U_c$ depends only *logarithmically* on the cut-off, its leading dependence on $t'$ remains unchanged and is thus exact. It is not clear at present whether the renormalization factor mentioned above remains finite also in $d = 2$.
[18] By this we mean a bandgap with nonzero wavevector difference between the valence band maximum and the conduction band minimum (see Fig. 2)
[19] W. Metzner, D. Vollhardt, Phys. Rev. Lett. **62** (1989) 324
[20] E. Müller-Hartmann, Z. Phys. B**74** (1989) 507
[21] A. Georges, G. Kotliar, W. Krauth, M. Rozenberg, Rev. Mod. Phys. **68** (1996) 13