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Superconductivity in weakly correlated electron systems

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Abstract. We study the influence of the short-ranged Hubbard correlation U between the conduction electrons on the Cooper pair formation in normal (s-wave) superconductors. The Coulomb correlation is considered within the standard second order perturbation theory, which becomes exact in the weak coupling limit but goes beyond the simple Hartree-Fock treatment by yielding a finite lifetime of the quasiparticles at finite temperature. An attractive pairing interaction V, which may be mediated by the standard electron-phonon mechanism, is considered between nearest neighbor sites. A critical value V_c for the attractive interaction is required to obtain a superconducting state. For finite temperature $T < T_c$ a gapless superconductivity is obtained due to the finite lifetime of the quasiparticles, *i.e.* the Coulomb correlation has a pair-breaking influence. The energy gap Δ and T_c depend very sensitively on U, V and band filling n and develop a maximum away from half filling as function of n. The ratio $2\Delta(0)/T_c$ varies with n, being higher than the BCS value near half filling and reaching the BCS value for lower n.

PACS. 74.20.Fg BCS theory and its development – 71.27.+a Strongly correlated electron systems; heavy fermions – 71.10.-w Theories and models of many electron systems

1 Introduction

We study an extended Hubbard model (EHM) with an on-site Coulomb repulsion U and an attractive inter-site interaction V, which is restricted to nearest neighbors only, for a review see reference [1]. The effects of inter-site pairing and the resulting anisotropy and symmetry of the superconducting order parameter have been investigated [2–9]. It has been shown that a BCS-like decoupling but with highly anisotropic pairing interaction may yield values of the ratio $2\Delta(0)/T_c$, which are much larger than the standard BCS value $2\Delta(0)/T_c = 3.53$ obtained for an isotropic ($\mathbf{k}$-independent) order parameter. In the existing literature on the EHM so far the Hubbard correlation has been treated within the standard Hartree-Fock approximation (HFA) [1,10], the Gutzwiller approximation[11] and the Hubbard decoupling schemes [12–14]. But it is well-known that for the simple Hubbard model [15–17] (without attractive pairing interaction) the HFA and the Hubbard decoupling have certain drawbacks; they do not properly reproduce important properties like quasi-particles with enhanced effective mass or the metal-insulator transition. The Gutzwiller approximation contains certain aspects of these properties at $T = 0$, as it yields a renormalized band and thus a mass enhancement and a metal-insulator transition, but it cannot account for finite-temperature effects. In this paper we apply the self-consistent second order perturbation theory (SOPT) to the extended Hubbard model. The SOPT can be considered to be the simplest systematic extension of the standard HFA, and it is a conserving approximation, which satisfies the Fermi liquid properties, and for the simple Hubbard model (without attractive pairing interaction) the SOPT becomes exact in the weak-coupling limit of small correlation U. It has been shown in recent years that many of the most essential properties are preserved, but practical calculations are greatly simplified, if models of correlated electron systems are studied within the limit of infinite dimensions, $d \to \infty$, introduced by Metzner and Vollhardt [18]; for an overview see reference [19]. These simplifications arise from the fact that the local approximation of a $\mathbf{k}$-independent self-energy becomes exact for $d \to \infty$ [20–23], because of which also the SOPT-calculations are much easier. By considering $1/d$-corrections it has also been shown for the simple Hubbard model that the results for $d = 3$ are almost identical to the results for $d \to \infty$ [24] so that a $d = \infty$ treatment is already sufficient to describe a three-dimensional system. Therefore, we restrict our SOPT-studies of the extended Hubbard model to infinite dimension, $d \to \infty$, which is justified at least for the purpose of a first model study. Thus we present here the first application of the self consistent SOPT, *i.e.* a systematic improvement of the HFA, to the extended Hubbard model with inter-site attraction and the first application of the – for correlated electron systems so successful and important – $d \to \infty$ limit to the EHM.

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2 Model

The Hamiltonian of the one band extended Hubbard model is given by

$$H = H_t + H_U + H_V, \tag{1}$$

with

$$H_t = t \sum_{\substack{\langle i,j \rangle \\ \sigma}} c^\dagger_{\mathbf{R}_i,\sigma} c_{\mathbf{R}_j,\sigma} - \mu \sum_{i,\sigma} n_{\mathbf{R}_i,\sigma} \tag{2}$$

$$H_U = \frac{U}{2} \sum_{i,\sigma} n_{\mathbf{R}_i,\sigma} n_{\mathbf{R}_i,-\sigma} \tag{3}$$

and

$$H_V = \frac{1}{2N} \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q} \\ \sigma,\sigma'}} V(\mathbf{q}) c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c^\dagger_{\mathbf{k}'-\mathbf{q},\sigma'} c_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma}. \tag{4}$$

Here $n_{\mathbf{R},\sigma} = c^\dagger_{\mathbf{R},\sigma} c_{\mathbf{R},\sigma}$ and H_t describes the conduction band with the energy dispersion $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$, where μ is the chemical potential. H_U denotes the on-site Coulomb-repulsion ($U > 0$) between two electrons of different spin at the same lattice site, and H_V is the attractive nearest neighbor ($V_{ij} < 0$) interaction. For a d-dimensional simple (hyper)-cubic lattice and the nearest neighbor tight-binding-approximation the conduction band dispersion reads: $\epsilon_{\mathbf{k}} = 2t\gamma_{\mathbf{k}}$ with $\gamma_{\mathbf{k}} = \sum_{i=1}^{d} \cos(k_i a)$, where a is the lattice constant, t denotes the hopping matrix element for nearest neighbours and d is the dimension. In the present paper, we make the approximation of a local (site-diagonal, *i.e.* **k**-independent) self-energy, which is correct in the limit $d \to \infty$. Consistent with this assumption is that the density of states per spin direction of the unperturbed noninteracting system has a Gaussian form [18,21]: $N^0(\omega) = 1/(\sqrt{2\pi}t^\star)\exp(-(\omega/t^\star)^2/2)$, where $t^\star$ is determined by the scaling of the hopping term (2) in the Hamiltonian H, so that the non-trivial limit is reached in infinite dimensions: $2t^2 d = t^{\star 2} = \text{const}$. We treat the attractive inter-site interaction (4) within the generalized Hartree-Fock decoupling with respect to anomalous expectation values

$$H_V \sim \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} V(\mathbf{k}-\mathbf{k}') \Big[\langle c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} \rangle c_{-\mathbf{k}',\downarrow} c_{\mathbf{k}',\uparrow} + \langle c_{-\mathbf{k}',\downarrow} c_{\mathbf{k}',\uparrow} \rangle c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} \Big], \tag{5}$$

and neglect normal expectation values for H_V, so that the decoupling corresponds to a BCS treatment. The extended s-wave part of the nearest neighbour pairing potential has the following form:

$$V(\mathbf{k}-\mathbf{k}') = \frac{2V_{\text{es}}}{d} \gamma_{\mathbf{k}} \gamma_{\mathbf{k}'}, \tag{6}$$

and consequently the energy gap $\Delta(\mathbf{k})$ has an extended s-wave character: $\Delta(\mathbf{k}) = \Delta_{\text{es}} \gamma_{\mathbf{k}}$. In the limit of infinite dimensions the strength of the attractive nearest neighbor interaction has to be scaled with $1/d$; this scaling makes the Hartree energy finite and all inter-site interactions can be treated in the Hartree approximation [21]. Furthermore the **k**-dependence of the anomalous Green function enters only *via* the dispersion $\epsilon_{\mathbf{k}}$ in $d \to \infty$, so that only pairing states having the symmetry of the lattice (extended s-wave symmetry) are possible [25]. For the on-site Coulomb repulsion H_U (3) we go beyond the standard Hartree-Fock (HF) approximation, since the on-site interaction remains dynamical in $d \to \infty$. In the HF analysis with $|V| \ll W$ (W bandwidth) simple s-wave superconductivity is possible only when $|V| > U$, which implies that in our mean field analysis the system will be superconducting only in the weak coupling regime ($U \ll W$). Then standard perturbation theory is applicable, and the simplest approximation beyond the (almost) trivial Hartree-Fock approximation is the second order perturbation treatment (SOPT) in the Coulomb correlation U.

In the large-d limit the site-diagonal (k-diagonal) SOPT selfenergy is explicitely given by [22]

$$\Sigma(x+\mathrm{i}y) = Un - \mathrm{i}\,\mathrm{sgn}(y) \frac{U^2}{N^2} \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-|y|t} \mathrm{e}^{\mathrm{i}\,\mathrm{sgn}(y)xt} \times \big\{ B(-\mathrm{sgn}(y)t) A^2(\mathrm{sgn}(y)t) + A(-\mathrm{sgn}(y)t) B^2(\mathrm{sgn}(y)t) \big\}, \tag{7}$$

with the definitions:

$$A(t) = -\frac{1}{\pi} \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{Im}\, G(x+\mathrm{i}0) f(x) \mathrm{e}^{-\mathrm{i}tx},$$
$$B(t) = -\frac{1}{\pi} \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{Im}\, G(x+\mathrm{i}0) \big[1-f(x)\big] \mathrm{e}^{-\mathrm{i}tx}, \tag{8}$$

where $f(\omega)$ denotes the Fermi- function and n the band-filling (*per* spin direction): $n_\uparrow = n_\downarrow = n$ and

$$G(z) = \frac{1}{N} \sum_{\mathbf{k}} G(\mathbf{k}, \mathbf{z})$$

is the on-site matrix element of the (normal) Green function.

In the present paper we neglect the isotropic s-wave pairing, which is unvavourable due to the on-site repulsive U, so that superconductivity in the isotropic s-wave channel is greatly reduced or even absent. Then in the presence of a nearest neighbor pairing the normal and the anomalous Green functions are given by:

$$G(\mathbf{k}, \mathrm{i}\omega_n) = \frac{\mathrm{i}\omega_n Z(\mathrm{i}\omega_n) + \xi_{\mathbf{k}} + \chi(\mathrm{i}\omega_n)}{[\mathrm{i}\omega_n Z(\mathrm{i}\omega_n)]^2 - [\xi_{\mathbf{k}} + \chi(\mathrm{i}\omega_n)]^2 - |\Delta_{\mathbf{k}}|^2}, \tag{9}$$

$$F(\mathbf{k}, \mathrm{i}\omega_n) = \frac{-\Delta_{\mathbf{k}}}{[\mathrm{i}\omega_n Z(\mathrm{i}\omega_n)]^2 - [\xi_{\mathbf{k}} + \chi(\mathrm{i}\omega_n)]^2 - |\Delta_{\mathbf{k}}|^2}, \tag{10}$$

where we have used the standard decomposition of the self-energy $\Sigma(\mathrm{i}\omega_n)$ into its even and odd part according to the relation $\Sigma(\mathrm{i}\omega_n) = \mathrm{i}\omega_n[1 - Z(\mathrm{i}\omega_n)] + \chi(\mathrm{i}\omega_n)$ so that $Z(\mathrm{i}\omega_n)$ and $\chi(\mathrm{i}\omega_n)$ both are even functions in the Matsubara frequency $\mathrm{i}\omega_n$

From this expression for the anomalous Green function we obtain the gap equation in the weak coupling regime

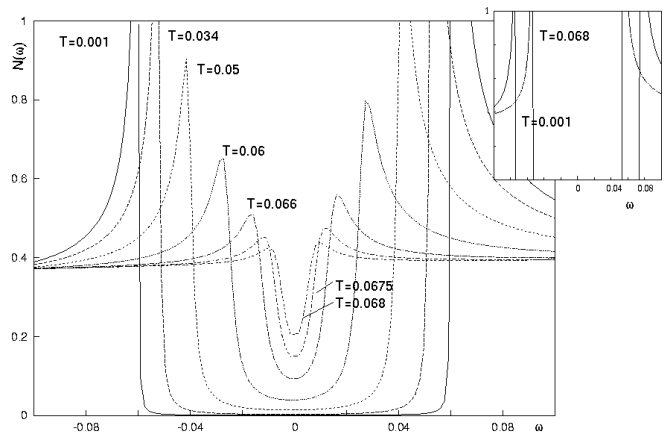

Fig. 1. Density of states $N(\omega)$ for different temperatures T as function of frequency ω for the Coulomb correlation $U = 1$, pairing interaction strength $V_{\rm es} = 2.4$ and band-filling $n = 0.4$. The inset shows corresponding HFA-results for $N(\omega)$.

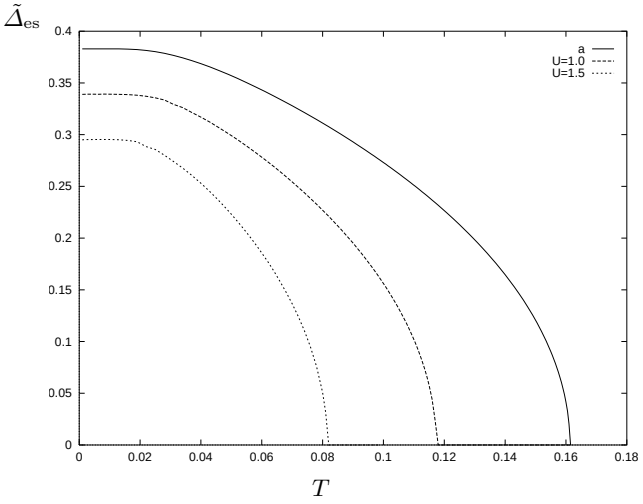

Fig. 2. Energy gap $\tilde{\Delta}_{\rm es}$ as function of temperature T for band-filling $n = 0.4$ and different values of $V = V_{\rm es}$. The solid curve indexed with (a) corresponds to the calculation in HF approximation.

$(U \ll W)$:

$$\frac{1}{|V_{\rm es}|/t^\star} = \frac{1}{t^\star\beta}\sum_n \int_{-\infty}^{\infty} {\rm d}\epsilon N^0(\epsilon) \times \frac{\epsilon^2}{[\omega_n Z({\rm i}\omega_n)]^2 + [\epsilon + \chi({\rm i}\omega_n) - \mu]^2 + |\tilde{\Delta}_{\rm es}/t^\star\epsilon|^2} \quad (11)$$

where we have introduced the scaled energy gap:

$$\tilde{\Delta}_{\rm es} = \sqrt{\frac{d}{2}}\Delta_{\rm es}. \quad (12)$$

In lowest (linear) order in U one gets $Z({\rm i}\omega_n) = 1$, and $\chi({\rm i}\omega_n) = Un$, which corresponds to the Hartree-Fock approximation for the repulsive correlation. Then we obtain the more familiar version of the gap equation:

$$\frac{1}{|V_{\rm es}|} = \frac{1}{t^{\star 2}}\int_{-\infty}^{\infty} {\rm d}\epsilon N^0(\epsilon)\epsilon^2 \times \frac{\tanh\left(\frac{\beta}{2}\sqrt{(\epsilon-\mu_{\rm eff})^2 + |\tilde{\Delta}_{\rm es}/t^\star|^2\epsilon^2}\right)}{2\sqrt{(\epsilon-\mu_{\rm eff})^2 + |\tilde{\Delta}_{\rm es}/t^\star|^2\epsilon^2}} \quad (13)$$

with an effective chemical potential $\mu_{\rm eff} = \mu - Un$.

3 Numerical results and discussion

For the numerical calculation we set the effective bandwidth $t^\star = 1$. In Figure 1 we present the density of states

$$N(\omega) = -\frac{1}{\pi}{\rm Im}G(\omega + {\rm i}0)$$

for different temperatures T as function of frequency ω for the Coulomb correlation $U = 1$, the pairing interaction strength $V_{\rm es} = 2.4$ and band-filling $n = 0.4$. Such a large value of V is needed to get superconducting solutions at all for this choice of the other parameters, because due to the anisotropy of the gap there exists a critical value $V_{\rm c}$, below which no superconductivity is possible. The critical value $V_{\rm c}$ does not depend on U in HFA, but it strongly depends on U in SOPT. The extended s-wave gap has nodes, *i.e.*, it vanishes for certain $\mathbf{k}$-points, and for half filling ($n = 0.5$) these nodes are on the Fermi surface. For this reason the extended s-wave superconductivity is always gapless, also for vanishing correlation U, for a half-filled band [26] and the critical $V_{\rm c}$ is largest and thus superconductivity is most unfavourable just for $n = 0.5$. For finite doping, however, *i.e.* away from half filling the nodes of $\Delta_{\mathbf{k}}$ are not on the Fermi surface and one obtains a superconducting gap [26] at least for zero temperature, as in Figure 1. But the density of states is gapless for finite temperatures T, in particular near the transition temperature $T_{\rm c}$, while it approaches a BCS-like density of states for $T \to 0$. This gapless behaviour is due to the pair breaking effect of the dynamical Coulomb correlations. A gapless density of states exists in SOPT, and it is a consequence of the finite imaginary part of the self-energy $\Sigma(z)$ at finite T, *i.e.*, of the quasiparticle damping. Thus the gapless superconductivity found here is a true correlation effect which is not obtained in the simple HFA. In HFA one gets a true gap also at finite $T < T_{\rm c}$, as can be seen from the inset in Figure 1, which shows the corresponding HFA-result for two temperatures $T < T_{\rm c}$.

In Figure 2 we present the order parameter $\tilde{\Delta}_{\rm es}$ as function of temperature. Near the transition temperature $\tilde{\Delta}_{\rm es}$ shows the typical BCS behaviour $\Delta(T) \sim \sqrt{1 - T/T_{\rm c}}$. By comparing with the corresponding HFA-result (curve a) we see that superconductivity is suppressed and becomes more unfavourable, if one treats the repulsive on-site correlation within a dynamical approximation like SOPT. Obviously the relative reduction of $T_{\rm c}$ is larger than the relative reduction of $\tilde{\Delta}_{\rm es}(T = 0)$ between HFA- and SOPT-result. Therefore, the ratio $\tilde{\Delta}_{\rm es}(T = 0)/T_{\rm c}$ is even larger within SOPT than the corresponding (already enlarged) HFA-result.

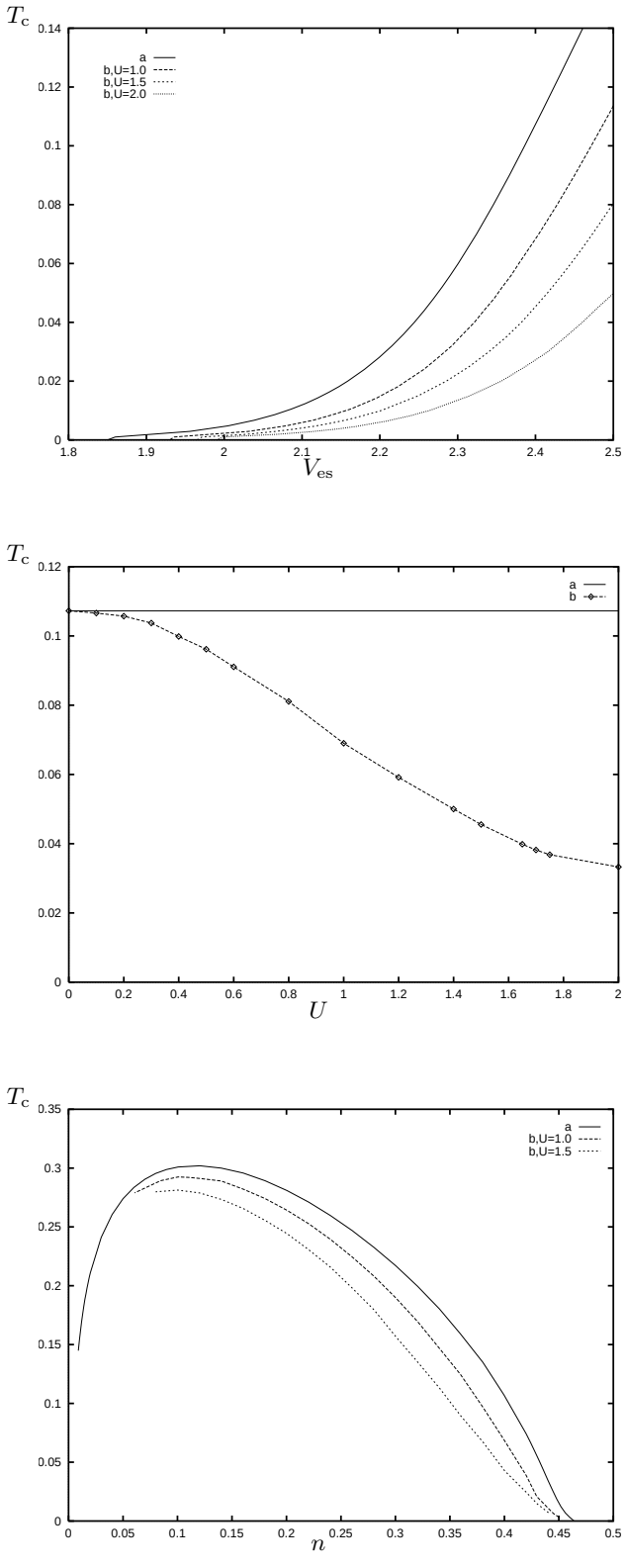

Fig. 3. Transition temperature T_c as a function of the pairing interaction V_{es} ($n = 0.4$), Coulomb correlation U ($n = 0.4, V_{es} = 2.4$) and as function of the band-filling n ($V_{es} = 2.4$). The curve (a) presents the calculation in HF approximation and the curve (b) the calculation with SOPT self-energy.

In Figure 3 we present the result for the transition temperature T_c as function of V_{es}, U and n. As expected similarly as the energy gap $\tilde{\Delta}_{es}$ also the transition temperature T_c increases with V_{es} (upper figure) and decreases with U (middle figure). From the lowest figure of Figure 3 we see that for this choice of $V = 2.4$ the transition temperature T_c becomes zero for band-filling $n > 0.45$, and the greatest reduction of T_c due to the Coulomb correlations occurs at a band-filling of $n \approx 0.35$. The transition temperature T_c is not a monotonous function of the band-filling n. T_c has its maximum at $n \approx 0.1$ and goes to zero for lower n. Near half-filling T_c is more strongly suppressed than the energy gap Δ_{es}.

In Figure 4 we show the dependence of the ratio $2\tilde{\Delta}_{es}(0)/T_c$ on U, V_{es} and n. We see that for low band-fillings the ratio has the BCS value and near half filling the ratio is enhanced. This enhancement of the ratio $2\tilde{\Delta}_{es}(0)/T_c$ is due to the strong anisotropy of the pairing interaction $V(\mathbf{k}-\mathbf{k}')$ and the dynamical Coulomb correlation U. The effect of the Coulomb correlation can be seen from the upper figure. The ratio $2\tilde{\Delta}_{es}(0)/T_c$ raises with increasing U. As function of the pairing interaction V_{es} for given U (middle figure) and band-filling n the ratio is zero unless $V_{es} > V_c$, and has a maximum at some $V > V_c$. The largest values obtained in SOPT for $2\tilde{\Delta}_{es}(0)/T_c$ are between 16 and 20, which exceeds the corresponding HFA-enhancement by a factor of almost 2.

4 Summary

To summarise, we have studied the extended Hubbard model with on-site repulsive interaction ($U > 0$) and additional attractive nearest neighbor interaction ($V < 0$). We treated the pairing interaction in the anomalous Hartree Fock (BCS) decoupling and the Coulomb correlations in the SOPT.

A critical value V_c of the inter-site interaction is required to obtain superconductivity at all, and this V_c depends strongly on the on-site correlation U. Furthermore, the energy gap and the critical temperature T_c depend strongly on the band filling. For half filling, for which the node in the extended-s-wave gap function is on the Fermi surface, superconductivity is strongly suppressed and exists only for very large values of $|V|$. But away from half filling a superconducting solution exists also for smaller values of V, and superconductivity is most favoured at a band filling of about $n \sim 0.1-0.2$. The ratio $2\Delta/T_c$ is strongly enhanced compared to the standard BCS result 3.53 up to values of about 15. The enhancement of the ratio $2\tilde{\Delta}_{es}/T_c$ is an effect of the strong anisotropy of the pairing interaction $V(\mathbf{k}-\mathbf{k}')$ and of the Coulomb correlation.

Furthermore, for finite temperature $0 < T < T_c$ we find gapless superconductivity away from half filling (*i.e.*, when the node in the gap function plays no role). This gapless superconductivity is a correlation effect and due to the finite imaginary part, *i.e.* the quasiparticle damping, obtained within the SOPT for finite T. Comparing our SOPT-results with corresponding HFA-results we find that the SOPT has a tendency to suppress

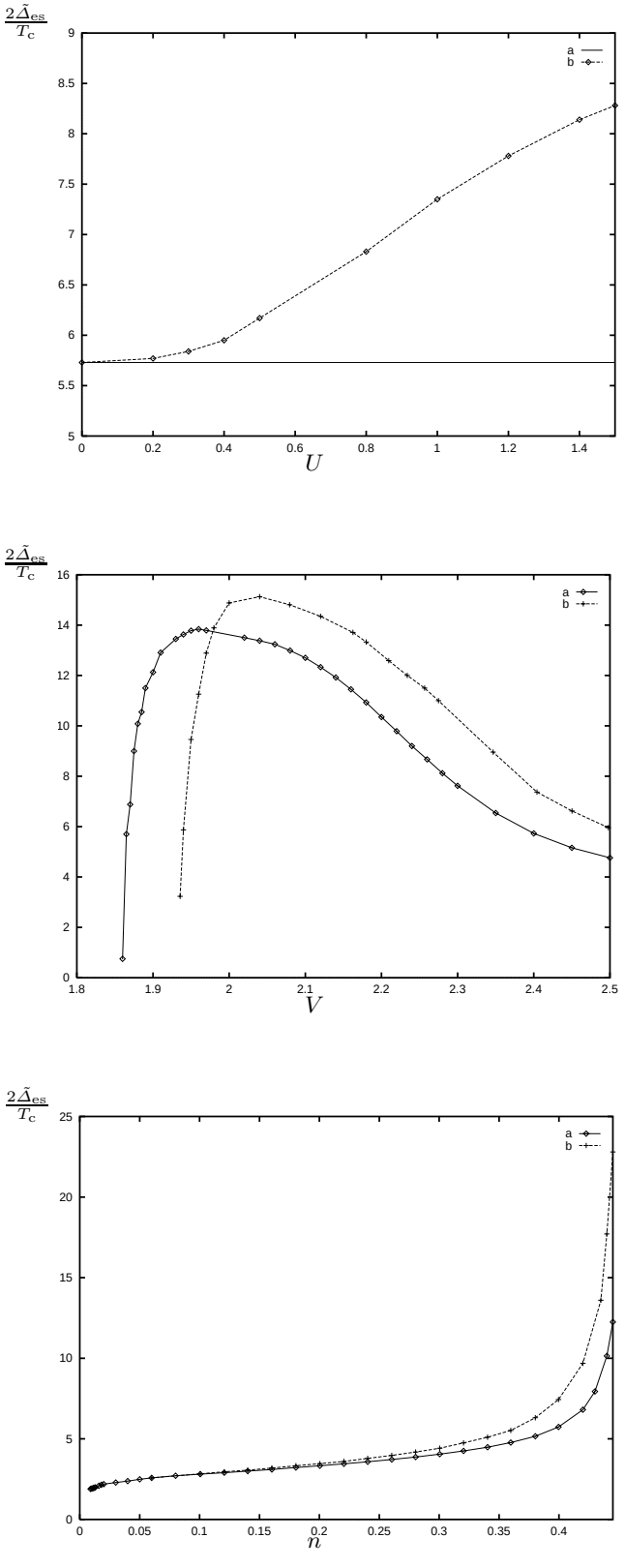

Fig. 4. Ratio $2\tilde{\Delta}(0)/T_c$ as a function of the U ($n = 0.4, V_{es} = 2.4$), V_{es} ($n = 0.4, U = 1$) and band-filling n ($U = 1, V_{es} = 2.4$). The curve (a) presents the calculation in HF approximation and the curve (b) the calculation with SOPT self-energy.

superconductivity: it yields quantitatively smaller values of the superconducting order parameter Δ and critical temperature T_c, and (in contrast to HFA) these values depend strongly on U. But the most important qualitative difference is the existence of superconductivity without a true gap for finite T in SOPT, *i.e.*, we obtain a gapless density of states for temperatures $0 < T < T_c$.

Our conclusion is that in the present model Coulomb correlations play an important role for the normal and the superconducting state, at least as far as temperatures near the transition temperature T_c are concerned.

Our model study shows that important qualitative and quantitative corrections have to be expected when treating the on-site correlation in a dynamical approximation like the SOPT beyond Hartree-Fock. Therefore, in the future such a dynamical treatment of the correlation should also be applied to the extended Hubbard model in realistic low dimension in which case one can also investigate a d-wave symmetry of the order parameter, which in $d \to \infty$ is impossible to describe.

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