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Phase diagrams of correlated electrons: systematic corrections to the mean field theory

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Abstract

Perturbative corrections to the mean field theory for particle–hole instabilities of interacting electron systems are computed within a scheme which is equivalent to the recently developed variational approach to the Kohn–Luttinger superconductivity. This enables an unbiased comparison of particle–particle and particle–hole instabilities within the same approximation scheme. A spin-rotation-invariant formulation for the particle–hole instabilities in the triplet channel is developed. The method is applied to the phase diagram of the t–t' Hubbard model on the square lattice. At the Van Hove density, antiferromagnetic and d-wave Pomeranchuk phases are found to be stable close to half filling. However, the latter phase is confined to an extremely narrow interval of densities and, away from the singular filling, d-wave superconducting instability dominates.

1. Introduction

In strongly correlated electron systems, several symmetry-breaking states usually appear as natural candidates for the ground state. This is so because, due to the large interaction strength, typically various mean field criteria for an instability are simultaneously satisfied. Unfortunately, mean field theory cannot tell reliably which of the possible competing instabilities wins. Therefore we are forced to look for finer methods, also taking into account the correlations that are neglected at the mean field level. The present paper is concerned with developing a systematic method that includes the dominant correlation effects neglected in the mean field theory. We require that the method satisfies the following criteria.

(i) As emphasized by Anderson [1], the energy of a quantum state is dominantly determined by its short-range correlations. Therefore, an unbiased comparison of different symmetry-breaking patterns requires that the same 'amount' of correlations is kept in all competing states. Obviously, mean field theory satisfies this criterion, neglecting the correlations in all states.

(ii) Long ago it has been shown that, when treated beyond the mean field level, even purely repulsive systems can support superconductivity [2]. We require that the general method reduces, in the case of superconductivity, to the recently developed perturbative scheme which enables a variational treatment of the Kohn–Luttinger superconductors [3].

Combining the above requirements, we are led to the search for a general lowest-order perturbative correction scheme to the mean field theory which treats all symmetry-breaking states on the same footing. This goal will be accomplished as follows. First, we choose the type of instability that we want to study. Then we split the Hamiltonian H of the interacting system into two parts. The first part contains the kinetic energy $H_0 = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k},\sigma}$ and that part H_1 of the interaction Hamiltonian that corresponds to a generalization of the reduced interaction Hamiltonian of the Bardeen–Cooper–Schrieffer (BCS) theory [4]. For instance, in the case of superconductivity, H_1 describes scattering of the Cooper pairs with zero total momentum or, in the case of magnetism, scattering of triplet particle–hole pairs with a given total momentum $\mathbf{q}$. Denoting the rest of the interaction Hamiltonian as H_2, the total Hamiltonian can be written as $H = H_0 + H_1 + H_2$.

As shown by Bogoliubov *et al* in the case of superconductivity [5], the mean field approach, when applied to the Hamiltonian $H_0 + H_1$, is essentially exact in the thermodynamic limit. In order to preserve this exactness, the term H_2, which describes scattering processes not included in the mean field theory, should be eliminated. Within our approach, this goal is achieved perturbatively. Namely, we construct a canonical transformation $\tilde{H} = \mathrm{e}^{\mathrm{i}S} H \mathrm{e}^{-\mathrm{i}S}$ which eliminates scattering processes to first order in the interaction strength. This is achieved for $H_2 + \mathrm{i}[S, H_0] = 0$ and the effective Hamiltonian reads, to second order in the interaction strength, as $\tilde{H} = H_0 + H_1 + \tilde{H}_2$, where $\tilde{H}_2 = [\mathrm{i}S, H_1 + H_2/2]$. The term $\tilde{H}_2$, which has replaced the term H_2 in the original Hamiltonian H, is typically even more complicated than H_2. So what have we gained? The key observation of our approach is that at weak coupling, $\tilde{H}_2$, being of second order in the coupling constant, is much smaller than H_2 and therefore can be treated in the mean field approximation. Note that this yields a nontrivial correction to the original mean field theory, because, in general, $\tilde{H}_2$ also contains terms of the type singled out into H_1. In order to better understand the last point, it is useful to observe that our approach is essentially variational, with a mean-field-type ansatz for the wavefunction $|\tilde{\psi}\rangle$ that minimizes the ground-state expectation value of the energy, $E = \langle\tilde{\psi}|\tilde{H}|\tilde{\psi}\rangle$. Equivalently, one can write $E = \langle\psi|H|\psi\rangle$ with $|\psi\rangle = \mathrm{e}^{-\mathrm{i}S}|\tilde{\psi}\rangle$ and interpret $|\psi\rangle$ as a mean field state written in terms of quasiparticles. In this language, it is not surprising that the effective interaction between the quasiparticles differs from the bare interaction.

The plan of the paper is as follows. In section 2 we construct the canonical transformation for the Hubbard model. We show explicitly that the effective Hamiltonian $\tilde{H}$ depends on the instability channel. It is worth pointing out that this is a common feature of our method and of various versions of the renormalization group approach to correlated electrons [6–10].

In section 3 we show how the method introduced in [3] fits the general scheme and we briefly review the main results of the method when applied to the superconducting instability.

In section 4 we develop the formalism for particle–hole instabilities with a finite total momentum of the particle–hole pairs. Our formulation allows for a simultaneous discussion of both the singlet and the triplet channels, the triplet channel being analysed within an explicitly spin-rotation-invariant formalism.

In section 5 we study particle–hole instabilities with a vanishing total momentum of the particle–hole pairs, called Pomeranchuk instabilities within Landau's Fermi liquid theory [11]. We simultaneously take into account the singlet and the triplet sectors, and also all point group symmetries, except for the identical representation in the singlet sector. For lattice models, this latter 'instability' is not associated with any symmetry breaking and simply corresponds to a change of the electron dispersion.

Finally, in section 6 we present the results of explicit calculations for the t–t' Hubbard model on the square lattice at electron densities ρ corresponding to the Van Hove filling of the noninteracting band, and we specialize to $\rho \sim 1$ and small t'/t.

2. Canonical transformation

For the sake of simplicity, let us proceed with an explicit evaluation of $\tilde{H}$ for the minimal microscopic model of interacting electrons, namely the Hubbard model. In that case, we can write

$$H_1 = \frac{U}{L}\sum_{\{123\}} c^\dagger_{3\uparrow}c_{1\uparrow}c^\dagger_{4\downarrow}c_{2\downarrow}\Delta_{1234},$$
$$H_2 = \frac{U}{L}\sum_{\{123\}} c^\dagger_{3\uparrow}c_{1\uparrow}c^\dagger_{4\downarrow}c_{2\downarrow}\left(1-\Delta_{1234}\right),$$

where L is the number of lattice sites and the summation index $\{123\}$ means momentum conservation $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4$. The cutoff function Δ_{1234} is always zero, except for the scattering processes which are to be singled out into H_1, in which case $\Delta_{1234} = 1$. For technical reasons, we also take $\Delta_{1234} = 1$ for processes which conserve the energy, i.e. if $\varepsilon_1 + \varepsilon_2 = \varepsilon_3 + \varepsilon_4$. This latter assumption will always be made in this paper and, for the sake of simplicity, it will not be mentioned explicitly in the formulae that follow.

One verifies readily that the canonical transformation we look for has the following Hermitian generator:

$$S = \frac{\mathrm{i}U}{L}\sum_{\{123\}}\frac{1-\Delta_{1234}}{\varepsilon_1+\varepsilon_2-\varepsilon_3-\varepsilon_4}c^\dagger_{3\uparrow}c_{1\uparrow}c^\dagger_{4\downarrow}c_{2\downarrow}. \tag{1}$$

It is worth pointing out that, for

$$\Delta_{1234} = \Delta_{2134} = \Delta_{1243}, \tag{2}$$

which will be always assumed from now on, the generator is explicitly spin-rotation invariant. A straightforward calculation shows that the effective scattering term $\tilde{H}_2$ is

$$\tilde{H}_2 = -\frac{U^2}{2L^2}\sum_{\{123\}}\sum_{\{\alpha\beta\gamma\}}\frac{(1-\Delta_{1234})(1+\Delta_{\alpha\beta\gamma\delta})}{\varepsilon_1+\varepsilon_2-\varepsilon_3-\varepsilon_4}[(\delta_{1\gamma}c^\dagger_{3\uparrow}c_{\alpha\uparrow}-\delta_{3\alpha}c^\dagger_{\gamma\uparrow}c_{1\uparrow})c^\dagger_{4\downarrow}c_{2\downarrow}c^\dagger_{\delta\downarrow}c_{\beta\downarrow}$$
$$+(\delta_{2\delta}c^\dagger_{4\downarrow}c_{\beta\downarrow}-\delta_{4\beta}c^\dagger_{\delta\downarrow}c_{2\downarrow})c^\dagger_{\gamma\uparrow}c_{\alpha\uparrow}c^\dagger_{3\uparrow}c_{1\uparrow}]. \tag{3}$$

Note that $\tilde{H}_2$ describes three-particle collisions and, as such (together with terms generated from higher orders of perturbation theory), allows for more complicated patterns of symmetry breaking than simple particle–particle or particle–hole condensates. Here we do not consider such possibilities.

In order to proceed, it is useful to specialize at this point to a particular symmetry-breaking channel. In this paper we will discuss three channels: (i) superconductivity with Cooper pairs with total momentum $\mathbf{q} = 0$, (ii) particle–hole pairs with a finite total momentum $\mathbf{Q}$, and (iii) particle–hole pairs with a vanishing total momentum $\mathbf{q} = 0$. It is also possible to apply our method to superconductivity with Cooper pairs with a nonvanishing total momentum, but we have not done so. As will become clear later, in each symmetry-breaking channel, there are singlet and triplet sectors in the spin space and various representations of the point group, therefore the number of different symmetry-breaking states is enormous.

3. Superconducting channel

This case has been discussed in detail in [3, 12–14], so the discussion will be very brief. According to the BCS theory [4], superconductivity can be viewed as an instability of the symmetric phase with respect to the formation of Cooper pairs with zero total momentum. Therefore in the superconducting channel, we choose

$$\Delta_{1234} = \begin{cases} 1 & \text{for } \mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4 = 0 \\ 0 & \text{otherwise.} \end{cases}$$

Taking the expectation value of $\tilde{H}$ in the superconducting state and introducing the angle-resolved pair field $b_{\alpha\beta}(\mathbf{k}) = \langle c_{-\mathbf{k}\alpha} c_{\mathbf{k}\beta} \rangle$, we have

$$E = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} f_{\mathbf{k}\sigma} - \frac{1}{2L} \sum_{\mathbf{k},\mathbf{p}} V^{\mathrm{sc}}_{\mathbf{kp}} b^*_{\alpha\beta}(\mathbf{k}) b_{\alpha\beta}(\mathbf{p}) + E_{\mathrm{FL}}, \tag{4}$$

where

$$E_{\mathrm{FL}} = \frac{U}{L}\frac{N^2}{4} + \frac{U^2}{L^2} \sum_{\{123\}} \frac{f_1 f_2 (1-f_3)(1-f_4)}{\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4}$$

is that part of the interaction energy which is not associated with symmetry breaking. Note that we have chosen an opposite sign convention for $V^{\mathrm{sc}}_{\mathbf{kp}}$ with respect to [3, 12–14]. In the present paper, attractive interactions are chosen to be positive. For exponentially small order parameters, which we expect in the region of validity of the present theory, we can neglect the change of E_{FL} between the symmetric and symmetry-broken state, and this term will not be discussed any more.

The pair scattering amplitude reads

$$V^{\mathrm{sc}}_{\mathbf{kp}} = -U - U^2 \chi'_{\mathrm{ph}}(\mathbf{k} + \mathbf{p}, \varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{k}}), \tag{5}$$

where $\chi'_{\mathrm{ph}}(\mathbf{q}, \omega)$ is the real part of the particle–hole susceptibility

$$\chi_{\mathrm{ph}}(\mathbf{q}, \omega) = \frac{1}{L} \sum_{\mathbf{K}} \frac{f_{\mathbf{K}} - f_{\mathbf{K}+\mathbf{q}}}{\varepsilon_{\mathbf{K}+\mathbf{q}} - \varepsilon_{\mathbf{K}} - \omega - \mathrm{i}0}. \tag{6}$$

The imaginary part of $\chi_{\mathrm{ph}}(\mathbf{q}, \omega)$ does not contribute to $V^{\mathrm{sc}}_{\mathbf{kp}}$, because the energy conserving processes are excluded from H_2. In the actual numerical implementation, we neglect the feedback effects on the susceptibility and replace the occupation numbers $f_{\mathbf{k}}$ by their values in the noninteracting system, $f^0_{\mathbf{k}}$. This replacement is again well controlled for exponentially small order parameters.

Following [15, 16], we introduce a 2×2 matrix notation $\hat{b}_{\mathbf{k}}$ for the pair field with the matrix elements $(\hat{b}_{\mathbf{k}})_{\alpha\beta} = b_{\alpha\beta}(\mathbf{k})$. Anticommutation of fermion operators then implies $\hat{b}_{-\mathbf{k}} = -\hat{b}^{\mathrm{T}}_{\mathbf{k}}$, where X^{T} is a matrix transposed to X. Let us further define the gap matrix $\hat{\Delta}_{\mathbf{k}} = \frac{1}{L}\sum_{\mathbf{p}} V_{\mathbf{kp}} \hat{b}_{\mathbf{p}}$ with the same symmetry properies as $\hat{b}_{\mathbf{k}}$ and introduce the following parameterization

$$\hat{\Delta}_{\mathbf{k}} = \begin{pmatrix} -d^1_{\mathbf{k}} + \mathrm{i}d^2_{\mathbf{k}}, & d^3_{\mathbf{k}} + d^0_{\mathbf{k}} \\ d^3_{\mathbf{k}} - d^0_{\mathbf{k}}, & d^1_{\mathbf{k}} + \mathrm{i}d^2_{\mathbf{k}} \end{pmatrix},$$

where a complex four-vector field $d^\nu_{\mathbf{k}} = (d^0_{\mathbf{k}}, \mathbf{d}_{\mathbf{k}})$ has been introduced that satisfies the conditions $d^0_{-\mathbf{k}} = d^0_{\mathbf{k}}$ and $\mathbf{d}_{-\mathbf{k}} = -\mathbf{d}_{\mathbf{k}}$.

States for which the vector function $\mathbf{q}_{\mathbf{k}} = d^0_{\mathbf{k}} \mathbf{d}^*_{\mathbf{k}} + (d^0_{\mathbf{k}})^* \mathbf{d}_{\mathbf{k}} + \mathrm{i}\mathbf{d}_{\mathbf{k}} \times \mathbf{d}^*_{\mathbf{k}}$ vanishes identically are called unitary [14] since, in that case, $\hat{\Delta}_{\mathbf{k}} \hat{\Delta}^\dagger_{\mathbf{k}}$ is proportional to a unit matrix. For unitary pairing states, the theory simplifies considerably and the self-consistent equations for the gap

function and the chemical potential μ, together with the expression for the ground-state energy, read as

$$\begin{aligned}\hat{\Delta}_{\mathbf{k}} &= \frac{1}{L}\sum_{\mathbf{p}} V^{\mathrm{sc}}_{\mathbf{kp}}\hat{\Delta}_{\mathbf{p}}\tanh\left(\frac{E_{\mathbf{p}}}{2T}\right),\\ N &= \sum_{\mathbf{k}}\left[1-\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\tanh\left(\frac{E_{\mathbf{k}}}{2T}\right)\right],\\ E_{\mathrm{GS}} &= -\sum_{\mathbf{k}}\frac{(E_{\mathbf{k}}-\xi_{\mathbf{k}})^2}{2E_{\mathbf{k}}}+\mu N,\end{aligned} \tag{7}$$

where $E_{\mathbf{k}} = (\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2)^{1/2}$ is the BCS quasiparticle energy, $|\Delta_{\mathbf{k}}|^2 = \sum_{\nu=0}^{3}|d^{\nu}_{\mathbf{k}}|^2$ is the spectroscopic gap, $\varepsilon_{\mathbf{k}}$ is the bare electron dispersion, and $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$.

4. Density wave channel

Next, we turn to the discussion of instabilities of the symmetric state with respect to the formation of bound particle–hole pairs with a nonvanishing total momentum $\mathbf{Q}$. The finite value of $\mathbf{Q}$ implies the presence of spatial modulations in the ground state, hence the name density wave channel. For the sake of simplicity, we specialize to the case when $2\mathbf{Q}$ is an inverse lattice vector. In particular, this is relevant for the t–t' Hubbard model at the Van Hove density, when the susceptibilities of the noninteracting system are singular at $\mathbf{Q} = (\pi, \pi)$ [17]. This latter case will be treated later as an explicit numerical example.

The key quantities describing the symmetry-broken phase are the angle-resolved particle–hole order-parameter fields $d^0_{\mathbf{k}} = 2^{-1}\sum_{\sigma}\langle c^{\dagger}_{\bar{\mathbf{k}}\sigma}c_{\mathbf{k}\sigma}\rangle$ and $\vec{d}_{\mathbf{k}} = 2^{-1}\sum_{\alpha\beta}\langle c^{\dagger}_{\bar{\mathbf{k}}\alpha}\vec{\sigma}_{\alpha\beta}c_{\mathbf{k}\beta}\rangle$, describing pairs with spin zero and spin one, respectively. Here we have introduced the abbreviation $\bar{\mathbf{k}} = \mathbf{k} + \mathbf{Q}$, and $\vec{\sigma}_{\alpha\beta}$ are the Pauli matrices. Let us notice that $d^0_{\bar{\mathbf{k}}} = (d^0_{\mathbf{k}})^*$ and $\vec{d}_{\bar{\mathbf{k}}} = (\vec{d}_{\mathbf{k}})^*$.

Next, we ask the question about the effective interactions in the density wave channel. In order to single out into H_1 those processes that scatter the particle–hole pairs with total momentum $\mathbf{Q}$, we have to choose

$$\Delta_{1234} = \begin{cases} 1 & \text{for } \mathbf{k}_3 - \mathbf{k}_1 = \mathbf{Q} \quad \text{or} \quad \mathbf{k}_3 - \mathbf{k}_2 = \mathbf{Q} \\ 0 & \text{otherwise.}\end{cases}$$

Note that this choice leads to a spin-rotation-invariant theory, since it satisfies the criterion equation (2).

Now let us calculate the expectation value of the Hamiltonian $\tilde{H}$ in a density wave state $|\tilde{\psi}_{\mathrm{dw}}\rangle$, $E = \langle\tilde{\psi}_{\mathrm{dw}}|\tilde{H}|\tilde{\psi}_{\mathrm{dw}}\rangle$. After a tedious but straightforward calculation, we find the result

$$E = \sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}}f_{\mathbf{k}\sigma} - \frac{1}{L}\sum_{\mathbf{k},\mathbf{p}}\left[V^{\mathrm{cdw}}_{\mathbf{kp}}d^0_{\mathbf{k}}d^0_{\mathbf{p}} + V^{\mathrm{sdw}}_{\mathbf{kp}}\vec{d}_{\mathbf{k}}\cdot\vec{d}_{\mathbf{p}}\right] + E_{\mathrm{FL}}, \tag{8}$$

in complete analogy with equation (4). The coefficients in front of the order parameter fields are the effective interactions that are sought. They read as

$$\begin{aligned}V^{\mathrm{cdw}}_{\mathbf{kp}} = {}& -U + \frac{U^2}{2}\left[\chi'_{\mathrm{pp}}(\mathbf{k}+\mathbf{p}, \varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{p}}) + \chi'_{\mathrm{pp}}(\mathbf{k}+\mathbf{p}, \varepsilon_{\bar{\mathbf{k}}}+\varepsilon_{\bar{\mathbf{p}}})\right]\\ & - U^2\left[\chi'_{\mathrm{ph}}(\mathbf{k}-\bar{\mathbf{p}}, \varepsilon_{\mathbf{k}}-\varepsilon_{\bar{\mathbf{p}}}) + \chi'_{\mathrm{ph}}(\bar{\mathbf{k}}-\mathbf{p}, \varepsilon_{\bar{\mathbf{k}}}-\varepsilon_{\mathbf{p}})\right],\end{aligned} \tag{9}$$

$$V^{\mathrm{sdw}}_{\mathbf{kp}} = U - \frac{U^2}{2}\left[\chi'_{\mathrm{pp}}(\mathbf{k}+\mathbf{p}, \varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{p}}) + \chi'_{\mathrm{pp}}(\mathbf{k}+\mathbf{p}, \varepsilon_{\bar{\mathbf{k}}}+\varepsilon_{\bar{\mathbf{p}}})\right], \tag{10}$$

where $\chi'_{\rm pp}(\mathbf{q},\omega)$ is the real part of the particle–particle susceptibility,

$$\chi_{\rm pp}(\mathbf{q},\omega)=\frac{1}{L}\sum_{\mathbf{K}}\frac{1-f^0_{\mathbf{K}}-f^0_{\mathbf{q}-\mathbf{K}}}{\varepsilon_{\mathbf{K}}+\varepsilon_{\mathbf{q}-\mathbf{K}}-\omega-\mathrm{i}0}. \tag{11}$$

Similarly, as in the discussion of the superconducting channel, the imaginary part does not enter due to the choice of Δ_{1234}, and the actual occupation numbers have been replaced by their noninteracting values. Note that, unlike in the superconducting case, the effective interactions are different in the singlet and triplet sectors.

Let us notice that both density wave interactions are real and have the following symmetries: $V_{\mathbf{kp}}=V_{\mathbf{pk}}=V_{\bar{\mathbf{k}}\bar{\mathbf{p}}}$. In analogy to the BCS theory, it is useful to introduce the gap functions $\Delta^0_{\mathbf{k}}=L^{-1}\sum_{\mathbf{p}}V^{\rm cdw}_{\mathbf{kp}}d^0_{\mathbf{p}}$ and $\vec{\Delta}_{\mathbf{k}}=L^{-1}\sum_{\mathbf{p}}V^{\rm sdw}_{\mathbf{kp}}\vec{d}_{\mathbf{p}}$. One verifies easily that $\Delta^0_{\bar{\mathbf{k}}}=(\Delta^0_{\mathbf{k}})^*$ and $\vec{\Delta}_{\bar{\mathbf{k}}}=(\vec{\Delta}_{\mathbf{k}})^*$. Let us define the auxiliary quantities $\delta_{\mathbf{k}}=(\varepsilon_{\mathbf{k}}-\varepsilon_{\bar{\mathbf{k}}})/2$ and $\omega_{\mathbf{k}}=(\varepsilon_{\mathbf{k}}+\varepsilon_{\bar{\mathbf{k}}})/2$ with the symmetry properties $\delta_{\bar{\mathbf{k}}}=-\delta_{\mathbf{k}}$ and $\omega_{\bar{\mathbf{k}}}=\omega_{\mathbf{k}}$, in terms of which the mean field Hamiltonian can be written in a compact form as

$$H=\sum_{\mathbf{k}}{}'(\hat{c}_{\mathbf{k}})^\dagger N_{\mathbf{k}}\hat{c}_{\mathbf{k}}+\sum_{\mathbf{k}}\left(d^0_{\mathbf{k}}\Delta^0_{\mathbf{k}}+\vec{d}_{\mathbf{k}}\cdot\vec{\Delta}_{\mathbf{k}}\right),$$

where the prime restricts the summation to only within the magnetic zone and $(\hat{c}_{\mathbf{k}})^\dagger=(c^\dagger_{\mathbf{k}\uparrow},c^\dagger_{\mathbf{k}\downarrow},c^\dagger_{\bar{\mathbf{k}}\uparrow},c^\dagger_{\bar{\mathbf{k}}\downarrow})$ is a four-component vector. Furthermore, we have introduced a 4×4 matrix $N_{\mathbf{k}}=\omega_{\mathbf{k}}\mathbf{I}+M_{\mathbf{k}}$, where $\mathbf{I}$ is a unit 4×4 matrix and

$$M_{\mathbf{k}}=\begin{pmatrix}\delta_{\mathbf{k}}\mathbf{1} & -(\Delta^0_{\mathbf{k}})^*\mathbf{1}-\vec{\Delta}^*_{\mathbf{k}}\cdot\vec{\sigma}\\ -\Delta^0_{\mathbf{k}}\mathbf{1}-\vec{\Delta}_{\mathbf{k}}\cdot\vec{\sigma} & -\delta_{\mathbf{k}}\mathbf{1}\end{pmatrix},$$

with $\mathbf{1}$ denoting a unit 2×2 matrix. Let us define the vector field $\vec{Q}_{\mathbf{k}}=\Delta^0_{\mathbf{k}}\vec{\Delta}^*_{\mathbf{k}}+(\Delta^0_{\mathbf{k}})^*\vec{\Delta}^\pm_{\mathbf{k}}$ $\mathrm{i}\vec{\Delta}_{\mathbf{k}}\times\vec{\Delta}^*_{\mathbf{k}}$. In analogy to the discussion of triplet superconductors, we will call states with $\vec{Q}_{\mathbf{k}}=0$ unitary. A major simplification is that, for unitary states, $M^2_{\mathbf{k}}$ is proportional to a unit matrix, $M^2_{\mathbf{k}}=E^2_{\mathbf{k}}\mathbf{I}$ with $E_{\mathbf{k}}=\sqrt{\delta^2_{\mathbf{k}}+|\Delta_{\mathbf{k}}|^2}$, where we have defined the spectroscopic gap $|\Delta_{\mathbf{k}}|^2=\sum_{\nu=0}^3|\Delta^\nu_{\mathbf{k}}|^2$. One checks easily that the eigenvectors of $M_{\mathbf{k}}$ are $E_{\mathbf{k}}$ and $-E_{\mathbf{k}}$, both of them being doubly degenerate. In what follows, we will develop an explicitly spin-rotation-invariant mean field theory for unitary states, closely following the standard treatment of triplet superconductivity [15, 16].

Let us assume that the unitary transformation $\hat{c}_{\mathbf{k}}=U_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}}$ from the bare electrons described by $(\hat{c}_{\mathbf{k}})^\dagger$ to the new quasiparticles described by $(\hat{\gamma}_{\mathbf{k}})^\dagger=(\gamma^\dagger_{\mathbf{k}\uparrow},\gamma^\dagger_{\mathbf{k}\downarrow},\gamma^\dagger_{\bar{\mathbf{k}}\uparrow},\gamma^\dagger_{\bar{\mathbf{k}}\downarrow})$ brings $N_{\mathbf{k}}$ to a diagonal form, $\tilde{N}_{\mathbf{k}}=U^\dagger_{\mathbf{k}}N_{\mathbf{k}}U_{\mathbf{k}}=\mathrm{diag}(E_{\mathbf{k}2},E_{\mathbf{k}2},E_{\mathbf{k}1},E_{\mathbf{k}1})$, where $E_{\mathbf{k}1}=\omega_{\mathbf{k}}+E_{\mathbf{k}}$ and $E_{\mathbf{k}2}=\omega_{\mathbf{k}}-E_{\mathbf{k}}$. Then the diagonalized Hamiltonian reads as

$$H=\sum_{\mathbf{k}\sigma}{}'\left[E_{\mathbf{k}2}\gamma^\dagger_{\mathbf{k}\sigma}\gamma_{\mathbf{k}\sigma}+E_{\mathbf{k}1}\gamma^\dagger_{\bar{\mathbf{k}}\sigma}\gamma_{\bar{\mathbf{k}}\sigma}\right]+\sum_{\mathbf{k}}\left(d^0_{\mathbf{k}}\Delta^0_{\mathbf{k}}+\vec{d}_{\mathbf{k}}\cdot\vec{\Delta}_{\mathbf{k}}\right),$$

and therefore $\langle\hat{\gamma}_{\mathbf{k}}(\hat{\gamma}_{\mathbf{k}})^\dagger\rangle=2^{-1}[\mathbf{I}+\tanh(\tilde{N}_{\mathbf{k}}/2T)]$. Transforming back to the $\hat{c}_{\mathbf{k}}$ operators, we thus have

$$\langle\hat{c}_{\mathbf{k}}(\hat{c}_{\mathbf{k}})^\dagger\rangle=U_{\mathbf{k}}\langle\hat{\gamma}_{\mathbf{k}}(\hat{\gamma}_{\mathbf{k}})^\dagger\rangle U^\dagger_{\mathbf{k}}=\frac{1}{2}\left[\mathbf{I}+\tanh\left(\frac{N_{\mathbf{k}}}{2T}\right)\right]. \tag{12}$$

Expanding the function $\tanh x$ into the Taylor series, making use of the binomial formula for powers of $N_{\mathbf{k}}=\omega_{\mathbf{k}}\mathbf{I}+M_{\mathbf{k}}$, and taking into account that $M^2_{\mathbf{k}}=E^2_{\mathbf{k}}\mathbf{I}$, we find

$$\tanh\left(\frac{N_{\mathbf{k}}}{2T}\right)=\frac{\mathbf{I}}{2}\left[\tanh\left(\frac{E_{\mathbf{k}1}}{2T}\right)+\tanh\left(\frac{E_{\mathbf{k}2}}{2T}\right)\right]+\frac{M_{\mathbf{k}}}{2E_{\mathbf{k}}}\left[\tanh\left(\frac{E_{\mathbf{k}1}}{2T}\right)-\tanh\left(\frac{E_{\mathbf{k}2}}{2T}\right)\right].$$

Inserting this result into equation (12) and comparing the components of the matrices on both sides, we find

$$n_{\mathbf{k}\sigma} = \frac{1}{2}\left[f_{\mathbf{k}1}\left(1+\frac{\delta_{\mathbf{k}}}{E_{\mathbf{k}}}\right)+f_{\mathbf{k}2}\left(1-\frac{\delta_{\mathbf{k}}}{E_{\mathbf{k}}}\right)\right],$$
$$n_{\bar{\mathbf{k}}\sigma} = \frac{1}{2}\left[f_{\mathbf{k}1}\left(1-\frac{\delta_{\mathbf{k}}}{E_{\mathbf{k}}}\right)+f_{\mathbf{k}2}\left(1+\frac{\delta_{\mathbf{k}}}{E_{\mathbf{k}}}\right)\right],$$
$$\vec{d}_{\mathbf{k}} = \vec{\Delta}^{*}_{\mathbf{k}}\frac{f_{\mathbf{k}2}-f_{\mathbf{k}1}}{E_{\mathbf{k}1}-E_{\mathbf{k}2}},$$
$$d^{0}_{\mathbf{k}} = (\Delta^{0}_{\mathbf{k}})^{*}\frac{f_{\mathbf{k}2}-f_{\mathbf{k}1}}{E_{\mathbf{k}1}-E_{\mathbf{k}2}},$$

and $\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}-\sigma}\rangle = 0$. In the above equations, we have used the notation $n_{\mathbf{k}\sigma} = \langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle$ and $f_{\mathbf{k}i} = f(E_{\mathbf{k}i}-\mu)$, where $f(x)$ is the Fermi–Dirac distribution function. Note that $f_{\bar{\mathbf{k}}i} = f_{\mathbf{k}i}$, since $E_{\bar{\mathbf{k}}i} = E_{\mathbf{k}i}$. From here, we finally find the self-consistent equations for the gap matrix and for the chemical potential, as well as the corresponding ground-state energy:

$$\vec{\Delta}_{\mathbf{k}} = \frac{1}{L}\sum_{\mathbf{p}} V^{\mathrm{sdw}}_{\mathbf{kp}}\vec{\Delta}^{*}_{\mathbf{p}}\frac{f_{\mathbf{p}2}-f_{\mathbf{p}1}}{E_{\mathbf{p}1}-E_{\mathbf{p}2}}, \tag{13}$$

$$\Delta^{0}_{\mathbf{k}} = \frac{1}{L}\sum_{\mathbf{p}} V^{\mathrm{cdw}}_{\mathbf{kp}}(\Delta^{0}_{\mathbf{p}})^{*}\frac{f_{\mathbf{p}2}-f_{\mathbf{p}1}}{E_{\mathbf{p}1}-E_{\mathbf{p}2}}, \tag{14}$$

$$N = \sum_{\mathbf{k}}[f_{\mathbf{k}1}+f_{\mathbf{k}2}],$$

$$E_{\mathrm{GS}} = \sum_{\mathbf{k}}\left[E_{\mathbf{k}1}f_{\mathbf{k}1}+E_{\mathbf{k}2}f_{\mathbf{k}2}+|\Delta_{\mathbf{k}}|^{2}\frac{f_{\mathbf{k}2}-f_{\mathbf{k}1}}{E_{\mathbf{k}1}-E_{\mathbf{k}2}}\right].$$

Note that the summations in these equations run over the full Brillouin zone. It should be stressed that the simple BCS-like form of equations (13), (14) is obtained only for unitary states with $\vec{Q}_{\mathbf{k}} = 0$.

In what follows, we do not allow for the simultaneous presence of charge and spin density wave order. Nevertheless, even with this simplification, the number of possible phases turns out to be quite large. For instance, on a square lattice, there are ten different symmetry-breaking patterns in the singlet sector, since $\Delta^{0}_{\mathbf{k}}$ may transform according to one of the five irreducible representations of the point group and there is an additional double degeneracy associated with the parity of the gap function under the translation in momentum space, $\mathbf{k} \to \bar{\mathbf{k}}$. Namely, if we decompose the order parameter to its real and imaginary parts, $\Delta^{0}_{\mathbf{k}} = x_{\mathbf{k}} + \mathrm{i}y_{\mathbf{k}}$, the gap equation can be written as

$$\begin{pmatrix} x_{\mathbf{k}} \\ y_{\mathbf{k}} \end{pmatrix} = \frac{1}{L}\sum_{\mathbf{p}} V^{\mathrm{cdw}}_{\mathbf{kp}}\begin{pmatrix} x_{\mathbf{p}} \\ -y_{\mathbf{p}} \end{pmatrix}\frac{f_{\mathbf{p}2}-f_{\mathbf{p}1}}{E_{\mathbf{p}1}-E_{\mathbf{p}2}}.$$

As observed by Hankevych and Wegner [10], the components with the symmetry properties $x_{\bar{\mathbf{k}}} = x_{\mathbf{k}}$ and $y_{\bar{\mathbf{k}}} = -y_{\mathbf{k}}$ are described by coupling constants with opposite signs.

As regards the triplet sector, based on the analogy of equation (13) with the triplet superconductor case [15, 16], we expect that, for degenerate representations of the point group, energy is minimized by Balian–Werthamer-like states involving complex patterns of $\vec{\Delta}_{\mathbf{k}}$. For square lattices to be studied explicitly in section 6, only the p representation is degenerate and, since that symmetry sector is not important in the range of parameters studied in section 6, in this paper we discuss only states of the type $\vec{\Delta}_{\mathbf{k}} = (x_{\mathbf{k}} + \mathrm{i}y_{\mathbf{k}})\vec{n}$, where $\vec{n}$ is a fixed direction in spin space and $x_{\mathbf{k}}$, $y_{\mathbf{k}}$ are real functions with the symmetry properties $x_{\bar{\mathbf{k}}} = x_{\mathbf{k}}$ and $y_{\bar{\mathbf{k}}} = -y_{\mathbf{k}}$.

Repeating the argument used already for the charge density waves, we again find that the components $x_{\mathbf{k}}$ and $y_{\mathbf{k}}$ are described by coupling constants with opposite signs.

5. Landau channel

In this section we consider instabilities of the high-temperature state with respect to the formation of bound particle–hole pairs with total momentum $\mathbf{q} = 0$. In this so-called Landau channel, we therefore choose

$$\Delta_{1234} = \begin{cases} 1 & \text{for } \mathbf{k}_3 = \mathbf{k}_1 \quad \text{or} \quad \mathbf{k}_3 = \mathbf{k}_2 \\ 0 & \text{otherwise.} \end{cases}$$

Let us introduce the angle-resolved singlet and triplet particle–hole fields, $n_{\mathbf{k}} = 2^{-1}\sum_\sigma \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle$ and $\vec{d}_{\mathbf{k}} = 2^{-1}\sum_{\alpha\beta}\langle c^\dagger_{\mathbf{k}\alpha}\vec{\sigma}_{\alpha\beta}c_{\mathbf{k}\beta}\rangle$, respectively. In terms of $n_{\mathbf{k}}$ and $\vec{d}_{\mathbf{k}}$, the expectation values of H_1 and $\tilde{H}_2$ read as

$$\langle H_1\rangle = \frac{U}{L}\sum_{\mathbf{kp}}\left[n_{\mathbf{k}}n_{\mathbf{p}} - \vec{d}_{\mathbf{k}}\cdot\vec{d}_{\mathbf{p}}\right],$$

$$\langle \tilde{H}_2\rangle = \frac{U^2}{L^2}\sum_{\{123\}}\frac{1-n_1-n_2}{\varepsilon_3+\varepsilon_4-\varepsilon_1-\varepsilon_2}\left[n_3n_4 - \vec{d}_3\cdot\vec{d}_4\right].$$

A crucial difference between the singlet and triplet fields is as follows. The triplet fields $\vec{d}_{\mathbf{k}}$ vanish in the symmetric high-temperature phase and we expect that, in the weak coupling limit, the development of a finite $\vec{d}_{\mathbf{k}}$ does not substantially change the electron distribution function. Therefore we can construct the triplet Landau interaction function as a second derivative of the interaction energy $\langle H_1 + \tilde{H}_2\rangle$ with respect to $\vec{d}_{\mathbf{k}}$. The derivatives can be evaluated for undeformed Fermi surfaces, leading to the result

$$V^{\mathrm{t}}_{\mathbf{kp}} = U - U^2\chi'_{\mathrm{pp}}(\mathbf{p}+\mathbf{k}, \varepsilon_{\mathbf{p}}+\varepsilon_{\mathbf{k}}). \tag{15}$$

Contrary to the triplet case, the singlet field $n_{\mathbf{k}}$ does not vanish, even in the noninteracting system. If we expand the interaction energy $\langle H_1 + \tilde{H}_2\rangle$ with respect to deviations of $n_{\mathbf{k}}$ from its value in the noninteracting system, besides quadratic terms, linear terms also appear in the deviation. Within the Landau Fermi liquid theory, this means that the quasiparticle dispersion relation is modified with respect to the bare spectrum. However, since in the discussion of superconductivity and of the density waves we have not taken into account the renormalization of the spectrum, in order to keep the same level of approximation we will consider only those singlet sector Landau instabilities that occur in the non s-wave channel, i.e. we assume that $n_{\mathbf{k}} = f^0_{\mathbf{k}} + d^0_{\mathbf{k}}$, where $f^0_{\mathbf{k}}$ is the noninteracting distribution and $d^0_{\mathbf{k}}$ transforms with respect to a nontrivial representation of the point group. With this restriction, the terms that are linear in $d^0_{\mathbf{k}}$ vanish, and we can write

$$E = \sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}}f_{\mathbf{k}\sigma} - \frac{1}{L}\sum_{\mathbf{k},\mathbf{p}}\left[V^{\mathrm{s}}_{\mathbf{kp}}d^0_{\mathbf{k}}d^0_{\mathbf{p}} + V^{\mathrm{t}}_{\mathbf{kp}}\vec{d}_{\mathbf{k}}\cdot\vec{d}_{\mathbf{p}}\right] + E_{\mathrm{FL}}, \tag{16}$$

where

$$V^{\mathrm{s}}_{\mathbf{kp}} = U^2\left[\chi'_{\mathrm{pp}}(\mathbf{p}+\mathbf{k}, \varepsilon_{\mathbf{p}}+\varepsilon_{\mathbf{k}}) - 2\chi'_{\mathrm{ph}}(\mathbf{p}-\mathbf{k}, \varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{k}})\right]. \tag{17}$$

Note that both in the singlet and in the triplet sectors, the interaction matrix is real and symmetric, $V_{\mathbf{kp}} = V_{\mathbf{pk}}$. After introducing the real gap functions $\Delta^0_{\mathbf{k}} = L^{-1}\sum_{\mathbf{p}} V^s_{\mathbf{kp}}d^0_{\mathbf{p}}$ and $\vec{\Delta}_{\mathbf{k}} = L^{-1}\sum_{\mathbf{p}} V^t_{\mathbf{kp}}\vec{d}_{\mathbf{p}}$, the mean field Hamiltonian can be written as

$$H = \sum_{\mathbf{k}}(\hat{c}_{\mathbf{k}})^\dagger\left[(\varepsilon_{\mathbf{k}} - \Delta^0_{\mathbf{k}})\mathbf{1} - \vec{\Delta}_{\mathbf{k}}\cdot\vec{\sigma}\right]\hat{c}_{\mathbf{k}} + \sum_{\mathbf{k}}\left[d^0_{\mathbf{k}}\Delta^0_{\mathbf{k}} + \vec{d}_{\mathbf{k}}\cdot\vec{\Delta}_{\mathbf{k}}\right],$$

where $(\hat{c}_{\mathbf{k}})^\dagger = (c^\dagger_{\mathbf{k}\uparrow}, c^\dagger_{\mathbf{k}\downarrow})$. Consider a unitary transformation $\hat{c}_{\mathbf{k}} = U_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}}$ to the quasiparticle operators $(\hat{\gamma}_{\mathbf{k}})^\dagger = (\gamma^\dagger_{\mathbf{k}-}, \gamma^\dagger_{\mathbf{k}+})$ with

$$U_{\mathbf{k}} = \frac{1}{\sqrt{2|\vec{\Delta}_{\mathbf{k}}|}} \begin{pmatrix} \sqrt{|\vec{\Delta}_{\mathbf{k}}| + \Delta^z_{\mathbf{k}}}, & -\sqrt{|\vec{\Delta}_{\mathbf{k}}| - \Delta^z_{\mathbf{k}}} \\ \frac{\Delta^x_{\mathbf{k}} + \mathrm{i}\Delta^y_{\mathbf{k}}}{\sqrt{|\vec{\Delta}_{\mathbf{k}}| + \Delta^z_{\mathbf{k}}}}, & \frac{\Delta^x_{\mathbf{k}} + \mathrm{i}\Delta^y_{\mathbf{k}}}{\sqrt{|\vec{\Delta}_{\mathbf{k}}| - \Delta^z_{\mathbf{k}}}} \end{pmatrix},$$

where we have introduced $|\vec{\Delta}_{\mathbf{k}}|^2 = \sum_{i=1}^3 (\Delta^i_{\mathbf{k}})^2$. One checks readily that the Hamiltonian is diagonal in the new basis,

$$H = \sum_{\mathbf{k}} \left[E_{\mathbf{k}-}\gamma^\dagger_{\mathbf{k}-}\gamma_{\mathbf{k}-} + E_{\mathbf{k}+}\gamma^\dagger_{\mathbf{k}+}\gamma_{\mathbf{k}+} + d^0_{\mathbf{k}}\Delta^0_{\mathbf{k}} + \vec{d}_{\mathbf{k}} \cdot \vec{\Delta}_{\mathbf{k}} \right],$$

with energy eigenvalues $E_{\mathbf{k}+} = \varepsilon_{\mathbf{k}} - \Delta^0_{\mathbf{k}} + |\vec{\Delta}_{\mathbf{k}}|$ and $E_{\mathbf{k}-} = \varepsilon_{\mathbf{k}} - \Delta^0_{\mathbf{k}} - |\vec{\Delta}_{\mathbf{k}}|$. Repeating the argument leading to equation (12), we find

$$\langle \hat{c}_{\mathbf{k}} (\hat{c}_{\mathbf{k}})^\dagger \rangle = U_{\mathbf{k}} \begin{pmatrix} 1 - f_{\mathbf{k}-} & 0 \\ 0 & 1 - f_{\mathbf{k}+} \end{pmatrix} U^\dagger_{\mathbf{k}}.$$

Making use of the formula $U_{\mathbf{k}}\sigma^z U^\dagger_{\mathbf{k}} = \vec{\sigma} \cdot \vec{\Delta}_{\mathbf{k}}/|\vec{\Delta}_{\mathbf{k}}|$, the right-hand side can be computed explicitly. Comparing the matrix elements of the left- and right-hand sides, we find

$$\vec{d}_{\mathbf{k}} = \vec{\Delta}_{\mathbf{k}} \frac{f_{\mathbf{k}-} - f_{\mathbf{k}+}}{E_{\mathbf{k}+} - E_{\mathbf{k}-}}, \qquad d^0_{\mathbf{k}} = \frac{1}{2}\left[f_{\mathbf{k}-} + f_{\mathbf{k}+} \right] - f^0_{\mathbf{k}}.$$

From here follow the self-consistent equations for the gap functions and the chemical potential, as well as the corresponding ground-state energy:

$$\vec{\Delta}_{\mathbf{k}} = \frac{1}{L} \sum_{\mathbf{p}} V^{\mathrm{t}}_{\mathbf{kp}} \vec{\Delta}_{\mathbf{p}} \frac{f_{\mathbf{p}-} - f_{\mathbf{p}+}}{E_{\mathbf{p}+} - E_{\mathbf{p}-}}, \tag{18}$$

$$\Delta^0_{\mathbf{k}} = \frac{1}{L} \sum_{\mathbf{p}} V^{\mathrm{s}}_{\mathbf{kp}} \left[\frac{1}{2}(f_{\mathbf{p}-} + f_{\mathbf{p}+}) - f^0_{\mathbf{p}} \right], \tag{19}$$

$$N = \sum_{\mathbf{k}} \left[f_{\mathbf{k}-} + f_{\mathbf{k}+} \right],$$

$$E_{\mathrm{GS}} = \sum_{\mathbf{k}} \left[\left(E_{\mathbf{k}-} + \frac{\Delta^0_{\mathbf{k}}}{2} \right) f_{\mathbf{k}-} + \left(E_{\mathbf{k}+} + \frac{\Delta^0_{\mathbf{k}}}{2} \right) f_{\mathbf{k}+} + |\vec{\Delta}_{\mathbf{k}}|^2 \frac{f_{\mathbf{k}-} - f_{\mathbf{k}+}}{E_{\mathbf{k}+} - E_{\mathbf{k}-}} \right].$$

We stress that equations (18) and (19) apply only if singlet channel Pomeranchuk 'instabilities' with s-wave symmetry are not allowed. In what follows, we specialize to pure singlet or pure triplet instabilities. Note that, as in section 4, for degenerate representations, nontrivial states in the triplet channel are likely, in which $\vec{\Delta}_{\mathbf{k}}$ does not preserve the same direction in spin space as one varies $\mathbf{k}$. Explicit examples of such states have been studied recently [18].

6. Application: t–t' Hubbard model at the Van Hove density

In the rest of this paper, we will study the phase diagram of the square lattice t–t' Hubbard model in the plane with the ordinates t'/t and electron filling ρ. In order to be able to also discuss the density wave states, we restrict ourselves to the so-called Van Hove line, i.e. to those combinations of t'/t and ρ that lead to a Fermi surface of the noninteracting system that crosses the saddle points of the dispersion at $(\pm\pi, 0)$ and $(0, \pm\pi)$. With this choice the most singular density wave susceptibility is expected at $\mathbf{Q} = (\pi, \pi)$ [17], satisfying the criterion that $2\mathbf{Q}$ is an inverse lattice vector.

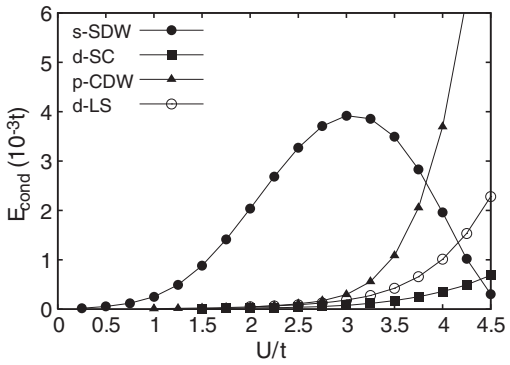

Figure 1. Condensation energy as a function of U at the Van Hove filling, $t'/t = 0$, $\rho = 1.0$, $L = 128$. The d-SC state is degenerate with d-SDW2 and d-CDW2 states.

All results reported in this section were obtained on $L \times L$ lattices with $L = 128$ sites and periodic boundary conditions. The susceptibilities entering the effective interactions have been written as convolutions and calculated using the fast Fourier transform (FFT) algorithm, as explained for the particle–hole case in [19]. In the time direction, we have sampled the interval $(0, \tau_{\max})$ with N points. Thus the energy precision is $\Delta\omega = 2\pi/\tau_{\max}$ and the maximal frequency is $\omega_{\max} = 2\pi N/\tau_{\max}$. In order that $\Delta\omega$ is comparable to the energy precision in $\mathbf{k}$-space, we require $\Delta\omega = 8t/L$. We also require $\omega_{\max} = 64t$ in order to faithfully describe the high-energy processes. This leads us to the choice $N = 8L = 1024$ time points and $\tau_{\max} = \pi L/(4t) = 32\pi/t$. In order to reduce the numerical error, the time evolution was damped according to $\exp(-\Gamma\tau)$ with $\Gamma = \Delta\omega/2 = t/32$. The accuracy of the FFT algorithm was checked by direct calculation of the susceptibilities. The self-consistent equations were solved by the damped iterative method. The condensation energy $E_{\text{cond}} = E_{\text{norm}} - E_{\text{GS}}$ was calculated as the difference between the energy of the symmetry-broken state E_{GS} and the normal-state energy $E_{\text{norm}} = 2\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} f^0_{\mathbf{k}}$. Note that stable states are described by a positive E_{cond}. In all figures, we plot the condensation energy per one lattice site.

In what follows, the symbols SC, CDW, SDW, LS, and LT stand for the superconducting, charge density wave, spin density wave, singlet Landau channel, and triplet Landau channel phases, respectively. Spatial representations of the point group of the square are denoted s, d, d_{xy}, and g (one-dimensional, even representations), and p (two-dimensional, odd representation). Note that we have not introduced separate symbols for singlet and triplet superconductors since, for superconductors, the spin sector is completely defined by the parity of the spatial representation. The density wave instabilities are characterized by an additional quantum number [10], namely the parity of the order parameter under translation in momentum space by $\mathbf{Q}$. Order parameters satisfying $\Delta_{\bar{\mathbf{k}}} = \Delta_{\mathbf{k}}$ and $\Delta_{\bar{\mathbf{k}}} = -\Delta_{\mathbf{k}}$ are distinguished by the suffix 1 and 2, respectively.

Our first task is to estimate the range of U where our theory is valid. To this end, it is useful to note that the effective interaction equations (5), (9), (10), (17) and (15), being functions of the particle–hole and particle–particle susceptibilities, are generically of the order U^2/t and exhibit only weak logarithmic singularities at isolated points, since the principal value integrals for $\chi(\mathbf{q}, \omega)$ in equations (6), (11) diverge only at special momenta and energies $\mathbf{q}, \omega$. From here, it follows that the contribution of the nontrivial order parameter to the ground-state energy equations (4), (8), and (16), being an integral over momentum space, is finite and of order U^2/t.

In order to estimate the region of validity of our theory explicitly, in figure 1 we plot the condensation energy as a function of U for $t'/t = 0$ and at half filling, $\rho = 1.0$. As

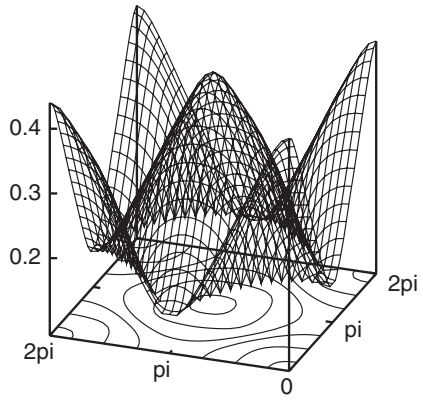

Figure 2. Gap function in the antiferromagnetic (s-SDW1) phase. The parameters are the same as in figure 1 and $U = 3t$.

expected, at weak coupling the leading instability is towards an s-SDW1 (antiferromagnetic) instability. Around $U \approx 3t$ the condensation energy of the antiferromagnetic state acquires a maximum. At larger coupling constants, different symmetry-breaking patterns dominate. Since the Hubbard model at half filling and $t'/t = 0$ is expected to order antiferromagnetically for all coupling constants [20], from figure 1 we estimate that our calculations are qualitatively correct up to $U \approx 3t$.

It should be noted that the overall shape of figure 1, and in particular the prediction of the relative stability of the phases, is in qualitative agreement with the calculation of the transition temperatures by the flow equation method by Hankevych and Wegner [10] (see their figure 1). The only qualitative difference with respect to [10] regards the relative stability of the d-LS (d-wave Pomeranchuk instability [21, 22]) and p-CDW2 (band splitting [10]) phases: according to our calculation, the p-CDW2 phase is more stable than the d-LS phase. Hankevych and Wegner also observed that, for $t'/t = 0$ and $\rho = 1.0$, there is an additional symmetry which guarantees that the d-SC state is degenerate with the d-SDW2 (triplet flux phase [23]) and d-CDW2 (singlet flux phase [23]) states. This degeneracy can also be proven within our formalism and is nicely satisfied by the data, thus providing a nontrivial check of the numerics.

Before proceeding, it is worth pointing out that the gap function in the simple antiferromagnetic (s-SDW1) phase is by no means featureless, as it would be in a mean field theory. Figure 2 shows that $\Delta_{\mathbf{k}}$ is suppressed along the underlying square Fermi surface, the suppression being largest close to the saddle points at $(\pm\pi, 0)$ and $(0, \pm\pi)$. This suppression is caused by the repulsive U^2 term in the effective interaction $V^{\mathrm{sdw}}_{\mathbf{kp}}$. Figure 1 shows that the repulsive term starts to dominate at $U > 3t$. A proper discussion of the spectroscopic implications of figure 2 would require also including the change of the normal-state dispersion (s-LS channel), which we have not attempted.

Summarizing the results at half filling, our data indicate that already at $U \approx 3t$, where our approach should still apply, there exist non-negligible tendencies towards ordering in several nontrivial symmetry-breaking states, many of which have been discussed extensively in the context of the physics of the cuprates: d-wave superconductivity, d-wave Pomeranchuk instability, and the flux phases (in the singlet case also called d-density wave phase [24]). In what follows, we discuss the evolution of these tendencies as we move along the Van Hove line towards smaller electron densities.

Inspection of figures 1 and 3–5 shows that the antiferromagnetic (s-SDW1) condensation energy rapidly diminishes with decreasing filling. This opens up the interesting possibility that

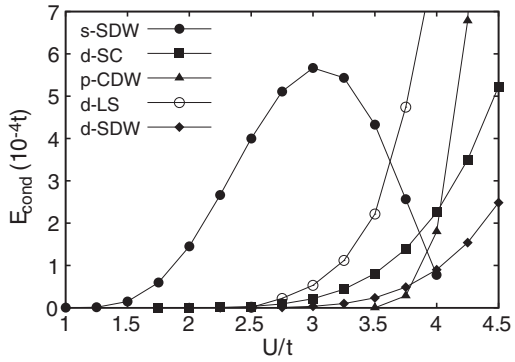

Figure 3. Condensation energy as a function of U at the Van Hove filling, $t'/t = 0.05$, $\rho = 0.959$, $L = 128$.

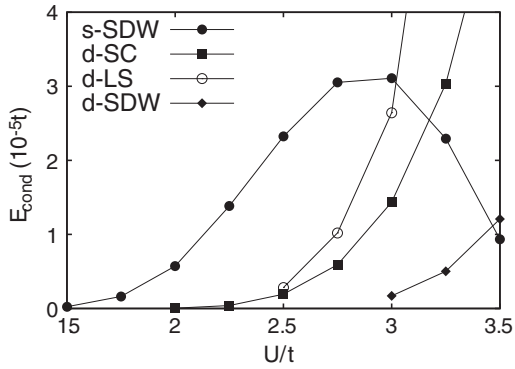

Figure 4. Condensation energy as a function of U at the Van Hove filling, $t'/t = 0.10$, $\rho = 0.918$, $L = 128$.

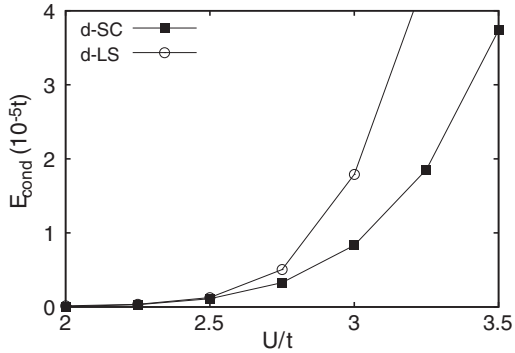

Figure 5. Condensation energy as a function of U at the Van Hove filling, $t'/t = 0.15$, $\rho = 0.875$, $L = 128$.

a nontrivial phase is stabilized at the Van Hove line. The leading subdominant instability at half filling is towards the band-splitting phase (p-CDW2). Figures 1, 3 and 4 show that this phase quickly loses stability and never becomes dominant in the region of applicability of our

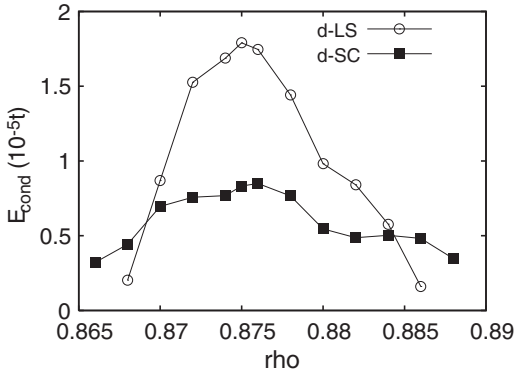

Figure 6. Condensation energy as a function of ρ in the vicinity of the Van Hove filling, $t'/t = 0.15$, $U = 3t$, $L = 128$.

method. Moreover, the degeneracy between the d-SC and the flux phases is lifted away from half filling: $E_{\rm cond}(\mathrm{dSC}) > E_{\rm cond}(\mathrm{dSDW2}) > E_{\rm cond}(\mathrm{dCDW2})$.

Thus we are led to a study of the competition between the antiferromagnet, the d-wave Pomeranchuk phase, and the d-wave superconductor. We find that, along the singular Van Hove line, the Pomeranchuk instability is stronger than the superconducting instability in the whole region that we have studied, i.e. up to $t'/t = 0.2$. Moreover, if we fix $U = 3t$ and consider the competition with the antiferromagnetic phase, we find that the d-wave Pomeranchuk phase becomes stabilized for $t'/t > (t'/t)_{\rm c} \approx 0.10$.

At the mean field level, the system at the Van Hove density is unstable towards antiferromagnetism for infinitesimal coupling. This raises the following interesting question: is it so that, at sufficiently weak coupling, when the mean field theory should apply, the system always has to order antiferromagnetically? Figures 1, 3, and 4 agree with this hypothesis. At smaller electron fillings we cannot confirm it, since for our lattice size we cannot reliably test states with small condensation energies.

Our results indicate that, at the Van Hove filling, the particle–hole instabilities are stronger than the superconducting ones. In the rest of this section, we wish to study the relative stability of phases away from the Van Hove filling. First we notice that, in regions of the t'/t versus ρ plane lying close to the Van Hove line, the density wave instabilities are expected to occur at wavevectors slightly different from $\mathbf{Q} = (\pi, \pi)$, and the formalism developed in section 4 does not apply. Therefore, in order to work in a region where the density wave instabilities are safely negligible, we have chosen to study the competition between the d-wave Pomeranchuk phase and the d-wave superconductor in the vicinity of the Van Hove point at $t'/t = 0.15$ for $U = 3t$. The results are shown in figure 6. As expected, sufficiently far away from the Van Hove filling (located at $\rho = 0.875$), the superconducting phase is stabilized. An unexpected feature of the data in figure 6 is that the d-wave Pomeranchuk phase is stable in an extremely narrow region around the Van Hove line even at moderate coupling $U = 3t$. As pointed out in [21], the d-LS Pomeranchuk instability does not cut off the Cooper channel singularity and therefore it is likely that that the true ground state in the vicinity of the Van Hove filling, besides breaking the rotational symmetry, is also superconducting.

7. Conclusions

In this work we have introduced a simple scheme which enables us to construct effective Hamiltonians for correlated electron systems in a controlled perturbative way. Our method

bears some similarity to Wegner's flow equations method [8, 10], which also performs a canonical transformation of the Hamiltonian. The main difference is that, in Wegner's approach, the resulting canonical transformation is a product of suitably chosen infinitesimal transformations, whereas our canonical transformation is generated by equation (1). It is worth pointing out that, in spite of this difference, the effective interactions derived by both methods are closely related. In fact, the flow equations method leads to the same effective interactions in the Landau channel as our equations (17), (15). Moreover, our result equation (5) for the Cooper channel reduces for on-shell processes, i.e. for Cooper pair scattering from $\mathbf{k}, -\mathbf{k}$ to $\mathbf{p}, -\mathbf{p}$ such that $\varepsilon_{\mathbf{k}} = \varepsilon_{\mathbf{p}}$, to the flow equation result [10]. Similarly, our effective interactions in the density wave channel equations (9), (10) reduce for on-shell processes, i.e. for scattering from $\mathbf{k}, \mathbf{p}$ to $\bar{\mathbf{k}}, \bar{\mathbf{p}}$ such that $\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{p}} = \varepsilon_{\bar{\mathbf{k}}} + \varepsilon_{\bar{\mathbf{p}}}$, to the corresponding flow equations formulae [10].

We have applied our method to the Hubbard model, but more complicated models can be also studied. As it stands, our scheme allows us to treat superconductivity, Pomeranchuk instabilities (except for the singlet instability transforming according to the trivial representation of the point group), and density wave instabilities with ordering wavevector $\mathbf{Q}$ (subject to the restriction that $2\mathbf{Q}$ is an inverse lattice vector). Both the singlet and the triplet sectors within each channel have been treated and it has been observed that, for degenerate representations, the phenomenology of the triplet particle–hole channels might be as rich as that of the triplet superconductors [15, 16].

An effective implementation of the method, making use of the fast Fourier transforms, has been developed. Lattices as large as 128×128 are tractable on PCs. The method has been applied to the phase diagram of the t–t' Hubbard model on the square lattice close to the Van Hove filling, for t'/t in the interval between 0 and 0.2. Our results are similar to those obtained using the flow equation method [10]: at the Van Hove line, particle–hole instabilities are found to dominate. The antiferromagnetic and the d-wave Pomeranchuk phases are stable for $t'/t < (t'/t)_c$ and $t'/t > (t'/t)_c$, respectively. The critical value of $(t'/t)_c$ depends on the value of the interaction strength U. The particle–hole instabilities are confined to an extremely narrow stripe of the t'/t versus ρ plane around the Van Hove line even at moderate coupling strength $U = 3t$, leaving most of the phase space to be dominated by the Kohn–Luttinger effect [2].

Straightforward future improvements of this work might include the study of larger systems and a finite-size scaling analysis of the results. The theory can be extended easily to finite temperatures. It is also possible to take into account the self-energy effects, or, in other words, the s-LS channel, and also the change of E_{FL} in the symmetry-breaking phases. Furthermore, the method can be applied to density wave states with more general wavevectors or to states with the simultaneous presence of symmetry breaking in different channels or symmetry sectors.

Turning to more speculative issues, an intriguing generalization would be to consider condensates of more than two particles or holes. A bosonic condensate would require a quadruplet of fields, and an inspection of equation (3) suggests that, in order to find the effective interaction for such processes, the perturbation expansion would have to be continued to higher orders. Finite lifetime effects should be studied as well. This might require a reorganization of perturbation theory in order to take into account the fact that the energy-conserving processes have been singled out into the tractable term H_1.

A serious limitation of our scheme is its inability to treat states without obvious order parameters, such as the Mott insulators. In such cases, the dynamical mean field theory (for a review, see [25]) seems to be the method of choice. On the other hand, for problems requiring a high resolution in momentum space, our method might be preferable.

Acknowledgments

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