Self Energy effect in frequency dependent Vertex flow equation

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I. INTRODUCTION

Introduction bla bla

II. FORMALISM

A. Model

The Hubbard model[1] describes spin-$\frac{1}{2}$ fermions with a density-density interaction:

$$\mathcal{H} = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \tag{1}$$

where $c^\dagger_{i,\sigma}$ and $c_{i,\sigma}$ are, respectively, creation and annihilation operators for fermions with spin $\sigma =\uparrow,\downarrow$. We consider the two-dimensional case with square lattice and repulsive interaction $U > 0$ at finite temperature T and in the SU(2) spin-symmetric phase. The hopping amplitude is restricted to $t_{ij} = t$ for nearest neighbors, $t_{ij} = t'$ for next-to-nearest neighbors.

B. Flow equations

In the following paragraph we will give some details about the functional renormalization group[2,3], and we will clarify some notation issue about the vertex.

Generally speaking, the fRG allows to use the renormalization group idea in the functional integral formalism. This is done by endowing the non-interacting propagator G_0, and hence the action, with an additional dependence on a scale parameter Λ, which generates an exact functional flow equation[4] with known initial conditions. The final result is recovered for some final Λ-value so that: $G_0^{\Lambda_f} = G_0$.

We will apply this approach to the effective action, whose expansions into the fields generates the one-particle irreducible (1PI) functions. By expanding the functional flow equation, one obtains a hierarchy of flow equations for the 1PI functions, involving vertexes of arbitrarily high orders. We will restrict ourselves to the two-particle level truncation by retaining only the two lowest nonvanishing orders in the expansion, i.e., we consider the flow of the self-energy Σ^Λ and of the two-particle 1PI vertex V^Λ, neglecting the effects of higher order vertexes. This truncation restricts the applicability of the approach to the weak-to-moderate coupling regime[5]. It can be furhter shown that, at the two-particle level truncaion, the fRG sums up efficiently, although approximately, the so-called parquet-diagrams[6–8].

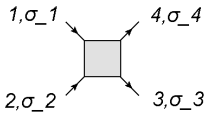

Figure 1: Notation of the two-particle vertex.

Due to translational invariance, we use the energy and momentum conservation to fix one of the arguments of the self-energy and of the vertex. Due to SU(2) symmetry, for the self-energy we only need to consider one function depending on one frequency-momentum argument:

$$\Sigma^\Lambda_{\sigma\sigma'}(k) = \Sigma(k)\delta_{\sigma,\sigma'}, \tag{2}$$

where $k = (\nu, \mathbf{k})$, ν is a fermionic Matsubara frequency and $\mathbf{k}$ a momentum in the first Brillouin zone.

For the notation of the two-particle vertex function $V_{\sigma_1,\sigma_2,\sigma_3,\sigma_4}(k_1, k_2, k_3)$ we refer to Fig. 1, where $k_i = (\nu_i, \mathbf{k_i})$. The momentum $k_4 = k_1 + k_2 - k_3$ is fixed by the other three and does not need to be specified. Furthermore SU(2)-symmetry guarantees that the vertex does not vanish only for six spin combinations[9]: $V^\Lambda_{\uparrow\uparrow\uparrow\uparrow} = V^\Lambda_{\downarrow\downarrow\downarrow\downarrow}$, $V^\Lambda_{\uparrow\downarrow\uparrow\downarrow} = V^\Lambda_{\downarrow\uparrow\downarrow\uparrow}$, and $V^\Lambda_{\uparrow\downarrow\downarrow\uparrow} = V^\Lambda_{\downarrow\uparrow\uparrow\downarrow}$. Finally, due to SU(2) symmetry and crossing relation one has:

$$\begin{aligned} V^\Lambda_{\uparrow\uparrow\uparrow\uparrow}(k_1,k_2,k_3) &= V^\Lambda_{\uparrow\downarrow\uparrow\downarrow}(k_1,k_2,k_3) \\ &\quad - V^\Lambda_{\uparrow\downarrow\uparrow\downarrow}(k_1,k_2,k_1+k_2-k_3), \qquad (3) \\ V^\Lambda_{\uparrow\downarrow\downarrow\uparrow}(k_1,k_2,k_3) &= -V^\Lambda_{\uparrow\downarrow\uparrow\downarrow}(k_1,k_2,k_1+k_2-k_3). \qquad (4) \end{aligned}$$

This allows us to consider only one function of three arguments for the vertex: $V^\Lambda(k_1, k_2, k_3) \equiv V^\Lambda_{\uparrow\downarrow\uparrow\downarrow}(k_1, k_2, k_3)$, all the others spin components being obtained by symmetry.

With these considerations the flow equation for the self energy[2] reads:

$$\frac{d}{d\Lambda}\Sigma^\Lambda(k) = -\int_p S^\Lambda(p)\left[2V^\Lambda(k,p,p) - V^\Lambda(k,p,k)\right], \tag{5}$$

with $p = (\omega, \mathbf{p})$ and $k = (\nu, \mathbf{k})$. We use the notation $\int_p = T\sum_\omega \int_{\mathbf{p}}$, $\int_{\mathbf{q}} = \int \frac{d\mathbf{q}}{4\pi^2}$ being the normalized integral over the first Brillouin zone.

$$S^\Lambda = \left.\frac{dG^\Lambda}{d\Lambda}\right|_{\Sigma=\text{const}} \tag{6}$$

is the single-scale propagator and $G^\Lambda = \left[(G_0^\Lambda)^{-1} - \Sigma^\Lambda\right]^{-1}$ is the full propagator.

The vertex flow equation[2,10] can be written as:

$$\frac{d}{d\Lambda}V^\Lambda(k_1,k_2,k_3) = \mathcal{T}^\Lambda_{\rm pp}(k_1,k_2,k_3) + \mathcal{T}^\Lambda_{\rm ph}(k_1,k_2,k_3) + \mathcal{T}^\Lambda_{\rm phc}(k_1,k_2,k_3), \tag{7}$$

where:[18]

$$\begin{aligned}
\mathcal{T}^\Lambda_{\rm pp}(k_1,k_2,k_3) &= -\frac{1}{2}\int_p \mathcal{P}^\Lambda(p,k_1+k_2-p)\Big\{V^\Lambda(k_1,k_2,k_1+k_2-p)V^\Lambda(k_1+k_2-p,p,k_3) \\
&\quad + V^\Lambda(k_1,k_2,p)V^\Lambda(p,k_1+k_2-p,k_3)\Big\}; \qquad (8)\\
\mathcal{T}^\Lambda_{\rm ph}(k_1,k_2,k_3) &= -\int_p \mathcal{P}^\Lambda(p,k_3-k_1+p)\Big\{2V^\Lambda(k_1,k_3-k_1+p,k_3)V^\Lambda(p,k_2,k_3-k_1+p) \\
&\quad - V^\Lambda(k_1,k_3-k_1+p,p)V^\Lambda(p,k_2,k_3-k_1+p) - V^\Lambda(k_1,k_3-k_1+p,k_3)V^\Lambda(k_2,p,k_3-k_1+p)\Big\}; \qquad (9)\\
\mathcal{T}^\Lambda_{\rm phc}(k_1,k_2,k_3) &= \int_p \mathcal{P}^\Lambda(p,k_2-k_3+p)V^\Lambda(k_1,k_2-k_3+p,p)V^\Lambda(p,k_2,k_3). \qquad (10)
\end{aligned}$$

Here we have defined the quantity:

$$\mathcal{P}^\Lambda(p,p') = G^\Lambda(p)S^\Lambda(p') + G^\Lambda(p')S^\Lambda(p). \tag{11}$$

For any Λ-dependence so that $G_0^{\Lambda_0} = 0$ the initial condition for the self-and the vertex are[2], respectively, $\Sigma^{\Lambda_0} = 0$ and $V^{\Lambda_0} = U$.

III. VERTEX APPROXIMATION

In order to deal with the frequency and momentum dependence of the vertex, we start by decomposing the vertex as follows:

$$V^\Lambda(k_1,k_2,k_3) = U - \phi^\Lambda_{\rm p}(k_1+k_2;k_1,k_3) + \phi^\Lambda_{\rm m}(k_3-k_1;k_1,k_2) + \frac{1}{2}\phi^\Lambda_{\rm m}(k_2-k_3;k_1,k_2) - \frac{1}{2}\phi^\Lambda_{\rm c}(k_2-k_3;k_1,k_2), \tag{12}$$

where the physical meaning of each ϕ channel will be understood by the structure of its flow equations:

$$\begin{aligned}
\dot\phi^\Lambda_{\rm p}(Q;k_1,k_3) &= -\mathcal{T}^\Lambda_{\rm pp}(k_1,Q-k_1,k_3), \qquad (13)\\
\dot\phi^\Lambda_{\rm c}(Q;k_1,k_2) &= -2\mathcal{T}^\Lambda_{\rm ph}(k_1,k_2,Q+k_1) \\
&\quad + \mathcal{T}^\Lambda_{\rm phc}(k_1,k_2,Q+k_1), \qquad (14)\\
\dot\phi^\Lambda_{\rm m}(Q;k_1,k_2) &= \mathcal{T}^\Lambda_{\rm phc}(k_1,k_2,Q+k_1), \qquad (15)
\end{aligned}$$

where $Q = (\Omega, \mathbf{Q})$ is a frequency and momentum transfer.

Following Refs. 10,11, we address first the momentum dependence. To this end, we introduce a decomposition of the unity by means of a set of orthonormal form factors for the two fermionic momenta $\{f_l(\mathbf{k})\}$ obeying the completeness relation:

$$\int_{\mathbf{k}} f_l(\mathbf{k}) f_m(\mathbf{k}) = \delta_{l,m}. \tag{16}$$

The procedure outlined here is described in detail, e.g., in Ref. 12

We can then project each channel on a subset of form factors, whose choice is physically motivated[10]. Let us stress that the if one could keep all the form factors the expansion would be exact.

For the pairing channel we keep only $f_s(\mathbf{k}) = 1$ and

$f_d(\mathbf{k}) = \cos k_x - \cos k_y$:

$$\phi_{\rm p}^{\Lambda}(Q;k_1,k_3) = \mathcal{S}_{\mathbf{Q}}^{\Omega;\nu_1,\nu_3} + f_d\left(\frac{\mathbf{Q}}{2}-\mathbf{k}_1\right) f_d\left(\frac{\mathbf{Q}}{2}-\mathbf{k}_3\right) \mathcal{D}_{\mathbf{Q}}^{\Omega;\nu_1,\nu_3}. \quad (17)$$

The divergence in the channel $\mathcal{S}$ is associated to s-wave superconductivity, while $\mathcal{D}$ to d-wave superconductivity.[2?]

For the charge and magnetic channels we restrict ourselves to $f_s(\mathbf{k}) = 1$ only:

$$\phi_{\rm c}^{\Lambda}(Q;k_1,k_2) = \mathcal{C}_{\mathbf{Q}}^{\Omega;\nu_1,\nu_2}, \quad (18)$$

$$\phi_{\rm m}^{\Lambda}(Q;k_1,k_2) = \mathcal{M}_{\mathbf{Q}}^{\Omega;\nu_1,\nu_2}, \quad (19)$$

corresponding to instabilities in the charge and magnetic channels, respectively (for notation simplicity we omit the Λ-dependences of the channel functions $\mathcal{S}$, $\mathcal{D}$, $\mathcal{C}$ and $\mathcal{M}$).

Let us stress that for each channel we have defined *its own* frequency notation, consisting of one transfer frequency in the specific channel and two remaining independent fermionic frequencies. At finite temperature these frequency transfer is a bosonic Matsubara frequency.
The choice of the mixed notation is the most natural[13] since the transferred momentum and frequency play a special role in the diagrammatics. Indeed, it is the only dependence generated in second order perturbation theory and the main dependence in finite order perturbation theory. This notation is also convenient to express the Bethe-Salpeter equations[9], which are deeply related to parquet-approximations and fRG.

Although one expects a leading dependence in the bosonic frequency, in particular in the weak coupling regime, we will see that in some cases the dependence on fermionic frequencies can become strong and not negligible.

In Refs. 10, whit a simplified frequency dependence, the channel functions above are interpreted as bosonic exchange propagators. Such an interpretation is missing with full frequency-dependence.

The flow equations for the channels $\mathcal{S}$, $\mathcal{D}$, $\mathcal{C}$ and $\mathcal{M}$ can be derived from the projection onto form factors of Eq. (8)-(10):

$$\dot{\mathcal{S}}_{\mathbf{Q}}^{\Omega;\nu_1,\nu_3} = -\int_{\mathbf{k}_1,\mathbf{k}_3} \mathcal{T}_{\rm pp}(k_1, Q-k_1, k_3); \quad (20)$$

$$\dot{\mathcal{D}}_{\mathbf{Q}}^{\Omega;\nu_1,\nu_3} = -\int_{\mathbf{k}_1,\mathbf{k}_3} f_d\left(\frac{\mathbf{Q}}{2}-\mathbf{k}_1\right) f_d\left(\frac{\mathbf{Q}}{2}-\mathbf{k}_3\right) \mathcal{T}_{\rm pp}(k_1, Q-k_1, k_3); \quad (21)$$

$$\dot{\mathcal{C}}_{\mathbf{Q}}^{\Omega;\nu_1,\nu_2} = \int_{\mathbf{k}_1,\mathbf{k}_2} \mathcal{T}_{\rm phc}(k_1,k_2,Q+k_1) - 2\mathcal{T}_{\rm ph}(k_1,k_2,k_2-Q); \quad (22)$$

$$\dot{\mathcal{M}}_{\mathbf{Q}}^{\Omega;\nu_1,\nu_2} = \int_{\mathbf{k}_1,\mathbf{k}_2} \mathcal{T}_{\rm phc}(k_1,k_2,Q+k_1). \quad (23)$$

The final equations are then obtained by substituting the decomposition (12) into the equations above, and using trigonometric equalities. As an example we report here the equation for the magnetic channel, while the expression for the other channels are reported in the Appendix:

$$\dot{\mathcal{M}}_{\mathbf{Q}}^{\Omega;\nu_1,\nu_2} = \sum_{\nu} L_{\mathbf{Q}}^{\Omega;\nu_1,\nu} P_{\mathbf{Q}}^{\Omega,\nu} L_{\mathbf{Q}}^{\Omega;\nu,\nu_2-\Omega}, \quad (24)$$

with:

$$P_{\mathbf{Q}}^{\Omega;\nu} = \int_{\mathbf{p}} G_{\mathbf{p}}^{\Lambda}(\omega) S_{\mathbf{Q}+\mathbf{p}}^{\Lambda}(\Omega+\omega) + G_{\mathbf{Q}+\mathbf{p}}^{\Lambda}(\Omega+\omega) S_{\mathbf{p}}^{\Lambda}(\omega), \quad (25)$$

and:

$$\begin{aligned} L_{\mathbf{Q}}^{\Omega;\nu_1,\nu_2} &= U + \mathcal{M}_{\mathbf{Q}}^{\Omega;\nu_1,\nu_2} \\ &+ \int_{\mathbf{p}} \Big\{ -\mathcal{S}_{\mathbf{p}}^{\nu_1+\nu_2;\nu_1,\nu_1+\Omega} \\ &-\tfrac{1}{2}\ \mathcal{D}_{\mathbf{p}}^{\nu_1+\nu_2;\nu_1,\nu_1+\Omega}[\cos(Q_x)+\cos(Q_y)] \\ &+\tfrac{1}{2}\ \left[\mathcal{M}_{\mathbf{p}}^{\nu_2-\nu_1-\Omega;\nu_1,\nu_2} - \mathcal{C}_{\mathbf{p}}^{\nu_2-\nu_1-\Omega,\nu_1,\nu_2}\right]\Big\} \end{aligned} \quad (26)$$

Let us notice that after the momentum integrals in P and L are performed, the right hand side can be expressed as a matrix-matrix multiplication in frequency space, where Ω and $\mathbf{Q}$ appear as parameters.

After this decomposition, the evaluation of vertex-flow equation, depending on six arguments, is reduced to the flow of the four functions $\mathcal{S}$, $\mathcal{D}$, $\mathcal{C}$, $\mathcal{M}$ each of them depending on three frequencies and one momentum only. In order to compute these equations numerically we needed to discretize the momentum dependence on patches covering the Brillouin zone and to truncate the frequency dependence to some maximal frequency value. More details about this are given in the Appendix.

Here let us stress, however, that an other approximation for the vertex function can be choosen, for instance approximating the frequency space with a single exchange bosonic frequency while keeping the dependence of all three momenta. We noted that, while the truncation of form factor expansion is well defined, in the case of single frequency approximation, the flow still depends on the two remaining frequencies, whose choice affects quantitatively and qualitatively the results.

A. Cutoff scheme

To use the flow equations defined above we need to specify the Λ-dependence of the non interacting propagator, often referred to as *cutoff scheme*, in connection to the scale-separation of the renormalization group. In the rest of the paper we have used two different cutoffs.

For most our calculations we have used the *Interaction cutoff*, introduced in Ref. 15:

$$G_0^{\Lambda}(k) = \Lambda G_0(k) = \frac{\Lambda}{i\nu - \mu - \varepsilon_{\mathbf{k}}}, \quad (27)$$

Where the scale-parameter Λ flows from 0 to 1, and with $\varepsilon_{\mathbf{k}} = -2t[\cos(k_x) + \cos(k_y)] - 4t' \cos(k_x)\cos(k_y)$. μ is the chemical potential needed to fix the occupation at a given value n. ν is a fermionic Matsubara-frequency: $\nu = \frac{\pi}{\beta}(2m+1)$, $m \in \mathbf{Z}$. $\beta = 1/T$ is the inverse temperature. Correspondingly the interacting Green's function reads:

$$G^{\Lambda}(k) = \frac{\Lambda}{i\nu - \varepsilon_{\mathbf{k}} - \mu^{\Lambda} - \Lambda\Sigma^{\Lambda}(k)} \tag{28}$$

We have introduced a Λ-dependent chemical potential to maintain the occupation fixed during the flow: the chemical potential becomes a functional of the flowing self-energy: $\mu^{\Lambda} = \mu[\Sigma^{\Lambda}]$, whose value is found by solving the equation:

$$n = n^{\Lambda} \equiv \int_k \frac{e^{i\nu 0^+}}{i\nu - \varepsilon_{\mathbf{k}} - \mu^{\Lambda} - \Lambda\Sigma^{\Lambda}(k)}. \tag{29}$$

The main advantage of the interaction cutoff is that the Λ-dependent action can be interpreted[15] as the physical action of the system with rescaled interaction $\tilde{U}^{\Lambda} = \Lambda^2 U$.

Since T acts as an infrared cutoff, for our purposes we do not need to worry about the fact that this cutoff is not scale-selective, and hence does not regularize possible divergences in the bubbles. Furthermore it has been shown in Ref. 16 that, in the context of the single-impurity Anderson model, the vertex-structures do not depend qualitatively on the cutoff-choice, and, at weak-coupling, depend on it only very little quantitatively.

As a benchmark for the robustness of our results on the cutoff-choice, we have used a soft version of the*frequency selective cutoff* defined[17] by:

$$G_0^{\Lambda}(k) = \frac{1}{i\mathrm{sign}\sqrt{\nu^2 + \Lambda^2} - \mu - \varepsilon_{\mathbf{k}}}, \tag{30}$$

with $\Lambda_0 = \infty$ and $\Lambda_{\mathrm{f}} = 0$. Also in this case we have performed our calculations at fixed occupation.

IV. RESULTS

A. Frequency dependence of Vertex

- Forward scattering problem seen by Salmhofer
- Show phase diagram, Λ_{cri} vs $x = 1 - n$, with and without Σ (for differenct t')
- Self energy "solve" the problem of charge instability.
- Suggestion: The charge problem exists also at van Hove filling where, according to the literature, the Σ has no effect when Karrasch approximation is taken into account.
- Colorplots: Mag and Charge channel

While much of the weak coupling momentum structure of the vertex (for the fermionic Hubbard model) is know by means of fRG, its frequency structure has been investigated much less. In recent years several results have been obtained for the single impurity Anderson model vertex, both on its own and as essential ingredient for diagrammatic extensions of DMFT. Citare: Rohringer, Kinza, Hafermann, Karrasch, Wentzell (and references therein) for the SIAM. Extensions of DMFT: DGA, DF, DMF2RG, Trilex, Quadrilex. However a systematic study keeping into account the full frequency dependence and a physically motivated approximation for the momentum dependence, and including fluctuations in all channels is still lacking.

In this persepctive we will present, in the next section, our results obtained by means of fully frequency dependent fRG. From the methodologic point of view, these results have to be considered as a proof of principle of the feasibility, and in some resepcts of the necessity, of a complete treatment of the frequency dependence of the vertex, with an impact on methods that aim at the study of strong coupling. From a more physical persepctive we will confirm some results already foreseen by 11 with a simpler frequency parametrization. However the study of the frequncy dependence of the verttex will allow us to gain a deeper understanding in these results, in particular the appearance of a *scattering instability*, and a sensitive reduction of the d-wave channel.

Furthermore, a frequency dependent vertex also allows us to compute the frequency dependent self energy, a task that, within fRG, requires heavier approximations whenver one restricts himself to a static vertex. We will show that the self-energy feedback in the flow equations is essential to guarantee the consistency between vertex and propagators in the flow equations. In fact, it turns out that even a Fermi-liquid self-energy can qualitatively change the physical results.

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B. Forward scattering problem

- Introduce perpendicular ladder (PL) for charge.
- Colorplot of charge in PL.
- Discuss the role of the Bubble at $\boldsymbol{Q} = (0,0)$ and plot it as a function of ν.

C. Self energy effects

- With self energy feedback, we didn't find any charge instability problem for any parameters range studied.
- Plot of the Fermi surface based patch scheme.
- Plot of $\Sigma(i\omega)$ at $\boldsymbol{k} = (\pi, 0)$, $\boldsymbol{k} = \boldsymbol{k}_{HS}$ and $\boldsymbol{k} = (\pi/2, \pi/2)$ in frequency space.

- Plot of $Z_{\boldsymbol{k}}$
- Plot of occupation with and without Σ

V. CONCLUSIONS

Conclusions...

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VI. APPENDICES

Appendices...

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[18] The equation for the particle-particle channel is slightly different from the one usually reported in fRG, see, e.g., Ref. 10. This is because we took $V^{\Lambda} = V^{\Lambda}_{\uparrow\downarrow\uparrow\downarrow}$ instead of $V^{\Lambda} = V^{\Lambda}_{\uparrow\downarrow\downarrow\uparrow}$.