On the fulfillment of Ward identities in the functional renormalization group approach

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I consider the fulfillment of conservation laws and Ward identities in the one- and two-loop functional renormalization group approach. It is shown that in a one-particle irreducible scheme of this approach Ward identities are fulfilled only with the accuracy of the neglected two-loop terms $O(V_{ab}^3)$ at one-loop order, and with the accuracy $O(V_{ab}^4)$ at two-loop order ($V_{ab}$ is the effective interaction vertex at scale $\Lambda$). The one-particle self-consistent version of the two-loop RG equations which leads to smaller errors in Ward identities due to the absence of the terms with non-overlapping loops, is proposed. In particular, these modified equations exactly satisfy Ward identities in the ladder approximation.

Strongly-correlated systems attract currently a lot of interest. While rigorous mathematical methods, such as the Bethe ansatz exist in one dimension, the consideration of systems with the dimensionality $d > 1$ requires certain approximations. These approximations can break conservation laws and therefore lead to results which are in contradiction with the conservation of particle number, momentum, energy, etc.

The fulfillment of Ward identities [1–3] guarantees the conservation of different quantities. Many years ago a way to construct conserving approximations was proposed by Baym and Kadanoff [4]. They have shown that the sufficient condition to fulfill conservation laws is the $\Phi$-derivability, which requires that for a given generating functional $\Phi[G]$ the self-energy $\Sigma$ and the two-particle vertex $\Gamma$ irreducible in the particle-hole channel satisfy

$$\Sigma = \delta \Phi / \delta G$$

and

$$\Gamma = \delta^2 \Phi / \delta G^2.$$ 

Later on, motivated by these ideas, Bickers and Scalapino [5] proposed the fluctuation exchange approximation (FLEX), which is based on a certain choice of $\Phi[G]$. This approximation has the advantage that it satisfies the conservation laws by construction. However, the disadvantage of FLEX is that the vertex $\Gamma = \delta \Sigma / \delta G$ which satisfies Ward identities is obtained only on the next level of approximation when the self-energy is already computed and therefore the calculation of the self-energy is performed with the vertices which do not satisfy Ward identities (see e.g. the discussion in Ref. [6]).

The situation is somewhat better in parquet-type approaches [7] (see also Refs. [8,9]). Both, vertex- and self-energy effects are accounted for in these approaches on the same ground. Although general $\Phi$-derivability of the parquet approach was recently proven in Ref. [10], the practical application of these approaches for systems with $d > 1$ meets serious computational difficulties and was performed only in a restricted number of cases [11,12].

Recently proposed functional renormalization group (RG) techniques, based on Polchinskii equations [13,14], Wick-ordered RG equations [15,16], and one-particle irreducible (1PI) RG equations [17–19], consider the self-energy and vertex corrections on the same footing, but require much smaller computational effort. These techniques were recently applied to the calculation of two-particle [14,18–21] and one-particle [22,23] properties of the two-dimensional Hubbard model, and to the impurity problem in a Luttinger liquid [24].

The fulfillment of Ward identities within the functional RG techniques is a non-trivial problem because of the use of different approximations: the truncation of an infinite hierarchy of RG equations (loop expansion), projection of the vertices on the Fermi surface etc. The main restriction comes from the loop expansion, used within these approaches. Unlike previous field-theoretical and Wilson RG approaches, not only singular, but also regular terms are accounted for in functional RG. This can lead to some inconsistencies and to the violation of Ward identities. Besides the approximations mentioned above, the introduction of the cutoffs in momentum or energy spaces can break Ward identities at the intermediate stages of the RG flow [25].

Therefore, it is useful to verify whether Ward identities are fulfilled in the functional RG approach. In the present paper I consider the fulfillment of Ward identities in one- and two-loop 1PI functional RG analysis without the projection of the vertices to the Fermi surface.

I consider a model with the action

$$S = \sum_k (i\nu_n - \varepsilon_k)c_k^{\dagger}c_k + \sum_{k_1...k_4,\sigma,\sigma'}\Gamma^0_{k_1,k_2;k_3,k_4}c_{k_1,\sigma}^\dagger c_{k_2,\sigma} c_{k_3,\sigma'} c_{k_4,\sigma'} \delta (k_1 + k_2 - k_3 - k_4)$$ (1)

with the general (frequency dependent) interaction

$$V^0_{k_1,k_2;k_3,k_4}; \hat{k}_i = (i\nu_n^{(i)}, k_i).$$

The conservation of charge leads to a continuity equation, which can be written in the continuum limit as

$$\mu J_q^\mu = 0,$$ (2)

$$J_q = \sum_{k,\sigma} \langle J_q \rangle_{k,\sigma} c_{k+q,\sigma}; J_q = \sum_{k,\sigma} \nabla \varepsilon_k \langle J_q \rangle_{k,\sigma} c_{k+q,\sigma} + J_q^{\text{int}},$$

where $\mu = 0...3$, $q = (\omega, q)$, $J_q^{\text{int}}$ is the contribution of electron-electron interaction to the current, $J_q^{\text{int}} = 0$ for a density-density interaction with $V^0_{k_1,k_2;k_3,k_4} = f(k_1 - k_3)$. The Ward identity which follows from (2) connects the one-particle self-energy $\Sigma_k$ with the charge- and charge-current vertices,
\[ \Gamma_{k,k';k+q,k'-q} = V_{k,k';k+q,k'-q} = \]
\[ G_k^{-1} G_k^{-1} G_k^{-1} G_{k+q}^{-1} G_{k'-q}^{-1} (T[c^\dagger_{k'}c_{q-k'} - q] G_{k+q})_{\text{ir}} \]
\[ \Gamma_{k,k';k+q,k'-q} = (\nabla_i \varepsilon_k) G_k^{-1} G_k^{-1} G_k^{-1} G_{k+q}^{-1} G_{k'-q}^{-1} (T[c^\dagger_{k'}c_{q-k'} - q] G_{k+q})_{\text{ir}} + \Gamma_{\text{int}}^i \]
where index \( \text{ir} \) stands for connected contributions, \( G_k \) is full one-particle Green function, \( \Gamma_{\text{int}}^i \) is the contribution to charge-current vertex produced by \( J_{\text{int}}^i \). The corresponding Ward identity for the model (1) reads (see Refs. [2,3,26] for a derivation)
\[ q \mu \sum_{k'} (-2 \Gamma_{\mu,k',k+q,k'-q}^\text{ir} + \Gamma_{\mu,k',k'-q,k+q}^\text{ir}) \times G_{k'} G_{k'-q} = \Sigma_k - \Sigma_{k+q}, \]
where \( \Gamma_{\mu} = (\Gamma_0, \Gamma) \).

The functional renormalization-group approach leads to an infinite hierarchy of differential equations for the self-energy \( \Sigma \), two-particle vertex \( V^{(4)} = V \), and higher-order vertices \( V^{(n)} \), \( n > 4 \). Truncated at the one-loop order, i.e. after neglect of \( V^{(n)} \) with \( n > 4 \) this hierarchy reduces to two integro-differential equations for the self-energy and the two-particle vertex, which in 1PI RG scheme [17,18] have the form
\[ \frac{d \Sigma_k}{d \Lambda} = V^A \circ \Sigma_k, \]  
\[ \frac{d V^A}{d \Lambda} = (G^A \circ \Sigma_k + \Sigma_k \circ G^A) \circ V^A. \]
In Eq. (5) \( \circ \) stands for the summation over intermediate moment-, frequency and spin-variables according to standard diagrammatic rules, \( \Lambda \) is the scaling parameter specified below. The initial condition for Eqs. (5) is \( \Sigma^{\Lambda_0} = 0, V^{\Lambda_0} = V_0 \) where \( \Lambda_0 \gg \max(|\varepsilon_k|) \). The propagators \( S, G \) are connected by
\[ S^A = -(G^A)^2 \frac{d}{d \Lambda}(G_0^A)^{-1}, \]
where \( G_0^A \) is the non-interacting Green function at scale \( \Lambda \). In particular, in the sharp momentum cutoff scheme [18,22] the propagators \( G^A \) and \( S^A \) are given by
\[ \left\{ \begin{array}{lcl}
G_k^A & = & \frac{1}{i \nu - \varepsilon_k - \Sigma_k^A} \% \%
S_k^A & = & \frac{\theta(|\varepsilon_k| - \Lambda)}{-\delta(|\varepsilon_k| - \Lambda)} \frac{1}{i \nu - \varepsilon_k - \Sigma_k^A}.
\end{array} \right. \]
in the sharp frequency cutoff scheme (at \( T = 0 \)) [24] by
\[ \left\{ \begin{array}{lcl}
G_k^A & = & \frac{\theta(|\nu| - \Lambda)}{-\delta(|\nu| - \Lambda)} \frac{1}{i \nu - \varepsilon_k - \Sigma_k^A}.
S_k^A & = & \frac{\theta(|\nu| - \Lambda)}{-\delta(|\nu| - \Lambda)} \frac{1}{i \nu - \varepsilon_k - \Sigma_k^A}.
\end{array} \right. \]
and in the temperature cutoff scheme [19] \( \Lambda = T \) and
\[ G_k^T = \frac{T^{1/2}}{i \nu - \varepsilon_k - \Sigma_k^T}, \quad S_k^T = \frac{1}{2} \frac{i \nu + \varepsilon_k}{(i \nu - \varepsilon_k - \Sigma_k^T)^2}. \]
Note that the results obtained in the present paper do not depend on the sharpness of the cutoff procedure in momentum or energy space and are valid for smooth cutoffs as well.

Consider first the Ward identity (4) for pure frequency shift \( q = (\omega, 0) \) within the momentum-cutoff RG approach (6). Written in differential form the corresponding identity reads
\[ \frac{\partial \Sigma_k}{\partial k_0} = \sum_{k'} (V_{k,k';k,k'} - 2V_{k,k';k,k'}) G_{k'}^2 \]
where \( k = (k_0, \vec{k}) \).

To verify whether this identity is satisfied at each intermediate scale \( \Lambda \) within the 1-loop RG scheme (5), one can use the following procedure: differentiate (9) with respect to \( \Lambda \) and compare with RG equations (5) differentiated with respect to \( k_0 \). The following identities are helpful when performing this procedure:
\[ \frac{\partial G_k^A}{\partial \Lambda} = S_k^A + (G_k^A)^2 \frac{\partial \Sigma_k^A}{\partial \Lambda}, \]
\[ \frac{\partial V^A}{\partial \Lambda} = -(G_k^A)^2 \frac{\partial \Sigma_k^A}{\partial \Lambda} \]
\[ \frac{\partial \Sigma_k}{\partial k_0} = -2G_k^A S_k^A (1 - \frac{\partial \Sigma_k}{\partial \Lambda} \frac{\partial \Lambda}{\partial k_0}). \]
In this way one finds that the identity (9) is satisfied if and only if
\[ \frac{\partial V_{k,k+q,k+q+k'}}{\partial k_0} = 2 \sum_p V_{k,k+p+k+p,k} V_{k+p,k+q+k+q+k+p} G_{k+p}^3 + 2 \sum_p (V_{k,k+p+k+p+k} - V_{k,k+p+k+q+k+p}) \]
\[ \times V_{k+p,k+q+k+q+k'} (G_{k+q+k+p}^2 G_{k+p} + G_{k+p}^2 G_{k+p}) \]
\[ + 2 \sum_p V_{k+p,k+q+k+q+k'} G_{k+p}^2 G_{k+p} G_{k+q-k+q} \]
\[ \frac{\partial \Sigma_{k+q+k+q+k'}}{\partial k_0} = 2 \sum_p G_{k+p+k+p} (V_{k,k+p+k+p,k} V_{k+p,k+q+k+q+k} + V_{k+p,k+q+k+q+k'} - 2V_{k,p+q+k+q+k'}) \]
\[ + \sum_p V_{k+p+k+p+k+q+k'}^2 G_{k+p+k+p} G_{k+p+k+q+k} \]
\[ + \sum_p V_{k+p+k+p+k+q+k'}^2 G_{k+p+k+p} G_{k+p+k+q+k} \]
\[ \frac{\partial V^A}{\partial \Lambda} = V^A \circ (G^A)^2 + (G^A)^2 \circ G^A \]
\[ = V^A \circ (G^A)^2 \circ V^A. \]
To see whether this equation is compatible with the RG equation for the vertex, Eq. (5b), one can differentiate Eq. (11) once more with respect to \( \Lambda \) and compare it with (5b) differentiated with respect to \( k_0 \). After long algebraic manipulations one obtains for the difference
\[ \frac{\partial}{\partial \Lambda} \left( \frac{\partial V_{k,k+q,k+q+k'}}{\partial k_0} \right) = \frac{\partial}{\partial k_0} \left( \frac{\partial V^A}{\partial \Lambda} \right) \]
Eq. (5b)
(and similar for $V_{k,k+q,k,k+q}^\Lambda$) two types of terms, which can be written in a short notation as

$$V \circ G^2 \circ \left(G^2 \circ \frac{d\Sigma}{d\Lambda} - S \circ \frac{d\Sigma}{dk_0}\right) \circ V + G^\Lambda \circ V^\Lambda \circ G^\Lambda \circ (G^\Lambda)^2 \circ V^\Lambda \circ S^\Lambda. \quad (13)$$

Both terms in Eq. (13) are of the order $O(V^3_{\Lambda})$ and closer inspection of these terms shows that the terms of each type do not cancel each other. Therefore, the momentum cutoff RG approach in one-loop approximation does not satisfy the Ward identity (9) exactly, but rather with the accuracy $O(V^3_{\Lambda})$. This accuracy is the same as the accuracy of the one-loop equations (5). The terms in Eq. (13) have different structures: in the terminology of Ref. [15] to find the bounds for the corresponding contributions responsible for the violation of the Ward identity.

Consider now the two-loop 1PI RG approach. The two-loop approximation corresponds to the inclusion of the contribution of the three-particle vertex $V^{(6)}_{\Lambda}$ up to the order $O(V^4_{\Lambda})$. The corresponding equations read

$$\frac{d\Sigma^\Lambda}{d\Lambda} = V^\Lambda \circ S^\Lambda \quad (14a)$$

$$\frac{dV^\Lambda}{d\Lambda} = V^\Lambda \circ (G^\Lambda \circ S^\Lambda + S^\Lambda \circ G^\Lambda) \circ V^\Lambda \quad (14b)$$

$$+ S^\Lambda \circ \int_\Lambda^{\Lambda_0} d\Lambda' \left(V^\Lambda \circ G^\Lambda \circ V^\Lambda \circ G^\Lambda \circ V^\Lambda \circ S^\Lambda\right)$$

$$+ S^\Lambda \circ \int_\Lambda^{\Lambda_0} d\Lambda' \left(V^\Lambda \circ (G^\Lambda)^2 \circ V^\Lambda \circ S^\Lambda \circ V^\Lambda\right)$$

where the last two lines of Eq. (14b) correspond to the vertex (Fig. 1a) and self-energy (Fig. 1b) corrections to the one-loop equations. Performing the same steps as for the one-loop approximation, we obtain a necessary condition to fulfill Ward identities:

$$\frac{\partial V^\Lambda}{\partial k_0} = V^\Lambda \circ \frac{\partial}{\partial k_0}(G^\Lambda \circ G^\Lambda) \circ V^\Lambda \quad (15)$$

Comparing again this equation with the RG equation for the vertex, Eq. (16b), one can observe that the equations are compatible with the accuracy $O(V^4_{\Lambda})$. As well as in the one-loop approximation, both types of terms, with overlapping and non-overlapping loops of order $O(V^4_{\Lambda})$, violate the Ward identity (9).

However the modification of Eqs. (14) with the last term replaced by its local-in-$\Lambda$ analog, i.e.

$$S^\Lambda \circ \int_\Lambda^{\Lambda_0} d\Lambda' \left(V^\Lambda \circ G^\Lambda \circ V^\Lambda \circ G^\Lambda \circ V^\Lambda \circ S^\Lambda\right) \to$$

$$S^\Lambda \circ V^\Lambda \circ (G^\Lambda \circ G^\Lambda) \circ V^\Lambda$$

leads to improvement in the fulfillment of the Ward identities. The corresponding equations read

$$\frac{d\Sigma^\Lambda}{d\Lambda} = V^\Lambda \circ S^\Lambda \quad (16a)$$

$$\frac{dV^\Lambda}{d\Lambda} = V^\Lambda \circ \left(\frac{d}{d\Lambda} (G^\Lambda \circ G^\Lambda) \circ V^\Lambda\right) \quad (16b)$$

$$+ S^\Lambda \circ \int_\Lambda^{\Lambda_0} d\Lambda' \left(V^\Lambda \circ G^\Lambda \circ V^\Lambda \circ G^\Lambda \circ V^\Lambda \circ S^\Lambda\right)$$

The difference between (14) and (16) is itself of the order $O(V^4_{\Lambda})$, i.e. of the order of the terms neglected in the two-loop approximation. The advantage of the modified two-loop RG equations, Eq. (16) is that they violate the Ward identity (9) by terms with overlapping loops only. Since such terms can correct only vertices but not the internal Green functions, one can consider Eqs. (16) as one-particle self-consistent. The absence of the terms with non-overlapping loops in the difference between the r.h.s. and the l.h.s. of the Ward identity (9) in this case is a consequence of the non-trivial cancellation between derivatives of the self-energy contained in the propagators of 1PI scheme (6) and the vertex corrections.

In particular, in the ladder approximation, when one selects only diagrams in the appropriate particle-hole channel and neglects the last term in the r.h.s. of Eq. (16b), Eqs. (16) take the form

$$\frac{d\Sigma^\Lambda}{d\Lambda} = V^\Lambda \circ S^\Lambda \quad (17a)$$

$$\frac{dV^\Lambda}{d\Lambda} = V^\Lambda \circ \left(\frac{d}{d\Lambda} (G^\Lambda \circ G^\Lambda) \circ V^\Lambda\right) \quad (17b)$$

These ladder equations differ from those in the one-loop approximation (5) only by the replacement $S^\Lambda \to dG^\Lambda/d\Lambda$ in the equation for the two-particle vertex and fulfill Ward identities exactly at any scale $\Lambda$. The solution of these equations leads to RPA-type vertices $V^\Lambda$, which satisfy standard integral equations.
\[ V_{kp,kp}^A = V_{kp,kp}^0 + \sum_{k'} V_{kk',kk'}^0 (G_k^A)^2 V_{kk',pp}^A \]
\[ V_{kp,kp}^A = V_{kp,kp}^0 + \sum_{k'} V_{kk',kk'}^0 (G_k^A)^2 V_{kk',pp}^A \]
\[ + \sum_{k'} (V_{kk',kk'}^0 - 2V_{kk',kk'}^0) (G_k^A)^2 V_{kk',pp}^A \] (18)

and the mean-field-type result for the self-energy,
\[ \Sigma_k^A = \sum_p (V_{kp,kp}^0 - 2V_{kp,kp}^0) G_p^A \] (19)
with the full (dressed) Green function \( G_A \). In the limit \( \Lambda \to 0 \) Eqs. (18) and (19) reduce to standard RPA and mean-field results, respectively.

For the non-ladder case and the regular curved Fermi surface one can use power counting arguments [15,17] to show that the equations (16) violate the Ward identity (9) by finite (non-divergent in the \( \Lambda \to 0 \) limit) terms \( O(V_A^4) \). One can expect that these equations will better satisfy Ward identities for both regular and singular Fermi surfaces due to the smallness of the contributions of the terms with overlapping loops [15]. Note that the replacement of the last term in Eq. (16) by its local analog and the additional replacement \( S_A \to dG_A/d\Lambda \) in the same term (which again produces finite errors of the order \( O(V_A^4) \)) can further improve the fulfillment of Ward identities. The analysis of this possibility requires however the consideration of the three-loop terms, which is beyond the scope of the present paper.

Therefore, in general, the momentum-cutoff RG scheme (6) at two-loop order satisfies the frequency component of the Ward identity (4) with the accuracy \( O(V_A^4) \). The same situation holds for the momentum component of the Ward identity (4) in the frequency cutoff RG approach, Eq. (7). The frequency component of the Ward identity (4) in frequency cutoff scheme and momentum component in momentum-cutoff scheme are violated because of additional terms coming from the differentiation of the cutoff functions [25]. At the same time, in the temperature cutoff RG scheme (8), which does not contain any cutoff in momentum or frequency space, similar calculations show that both, frequency- and momentum-components of the Ward identity are satisfied at two-loop order up to the same accuracy \( O(V_A^4) \).

In conclusion, we have considered the fulfillment of Ward identities in the one- and two-loop RG approach. The frequency components of Ward identities in the momentum-cutoff scheme and the momentum components in the frequency-cutoff scheme are generally satisfied up to terms of \( O(V_A^4) \) in the one-loop approximation and \( O(V_A^4) \) in the two-loop approximation. The one-particle self-consistent version of the two-loop RG equations (16) leads to smaller errors in the fulfillment of Ward identities due to absence of terms with non-overlapping loops. In the ladder approximation this version of the two-loop equations satisfies Ward identities exactly.

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