Ward identities for the Anderson impurity model:
derivation via functional methods and the exact
renormalization group

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Abstract

Using functional methods and the exact renormalization group we derive Ward
identities for the Anderson impurity model. In particular, we present a non-
perturbative proof of the Yamada–Yosida identities relating certain coefficients
in the low-energy expansion of the self-energy to the thermodynamic particle
number and spin susceptibilities of the impurity. Our proof underlines the
relation of the Yamada–Yosida identities to the \( U(1) \times U(1) \) symmetry
associated with the particle number and spin conservation in a magnetic field.

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1. Introduction

In quantum field theory symmetries and the associated conservation laws imply Ward identities,
which are the exact relations between different types of Green’s functions or vertex functions
[1]. The constraints imposed by the Ward identities can be very useful to devise accurate
approximation schemes which do not violate conservation laws. In this work, we present a
non-perturbative derivation of the Ward identities relating the coefficients in the low-frequency
expansion of the retarded self-energy \( \Sigma_\text{r}(\omega + i\delta) \) of the Anderson impurity model (AIM) to
certain thermodynamic susceptibilities. A perturbative derivation of these identities has first
been given by Yamada and Yosida [2]. For particle–hole symmetric filling and in the limit of
an infinite bandwidth of the conduction electron dispersion with flat density of states, these identities read

\[
\text{Re} \Sigma(\omega + i0) = \frac{U}{2} + \left( 1 - \frac{\tilde{\xi}_e + \tilde{\xi}_s}{2} \right) \omega + O(\omega^2), \quad (1.1)
\]

\[
\text{Im} \Sigma(\omega + i0) = -\left( \frac{\tilde{\xi}_e - \tilde{\xi}_s}{2} \right)^2 \frac{\omega^2}{2\Delta} + O(\omega^3). \quad (1.2)
\]

Here, \( U \) is the on-site interaction at the impurity site, \( \Delta \) is the imaginary part of the hybridization function in the limit of an infinite bandwidth of the conduction electron band and \( \tilde{\xi}_e \) and \( \tilde{\xi}_s \) are the dimensionless particle number (charge) and spin susceptibilities, which are defined in equations (4.34) and (4.35) below. A generalization of equations (1.1) and (1.2) to the AIM out of equilibrium can be found in [3].

Yamada and Yosida obtained the above identities by comparing the coefficients in the perturbation series of both sides of equations (1) and (2) to all orders in powers of \( U/\Delta \). An alternative derivation using diagrammatic techniques can be found in the book by Hewson [4]. Unfortunately, in both approaches the close relation of the above identities to the Ward identities non-perturbatively are well known [1], apparently there exists no derivation in the literature using these functional methods. In this work, we present such a non-perturbative proof of equations (1) and (2) by combining standard functional techniques [1] with certain exact relations between the derivatives of the self-energy with respect to frequency, chemical potential and magnetic field which we derive within the framework of the exact renormalization group [5, 6].

To set the stage for our calculation and to define our notation, let us recall that the single-site AIM is defined in terms of the following second-quantized Hamiltonian:

\[
\hat{H} = \sum_{k\sigma} (\epsilon_k - \sigma h) \hat{c}^{\dagger}_{k\sigma} \hat{c}_{k\sigma} + \sum_{\sigma} (E_d - \sigma h) \hat{d}^{\dagger}_{\sigma} \hat{d}_{\sigma} + U \sum_{d} \hat{d}^{\dagger}_{\uparrow} \hat{d}_{\uparrow} \hat{d}^{\dagger}_{\downarrow} \hat{d}_{\downarrow} + \sum_{k\sigma} \left( V_k \hat{d}^{\dagger}_{\sigma} \hat{c}_{k\sigma} + V_k \hat{c}^{\dagger}_{k\sigma} \hat{d}_{\sigma} \right),
\]

where \( \hat{c}_{k\sigma} \) annihilates a non-interacting conduction electron with momentum \( \mathbf{k} \), energy dispersion \( \epsilon_k \) and spin projection \( \sigma \), while the operator \( \hat{d}_{\sigma} \) annihilates a localized correlated \( d \)-electron with the atomic energy \( E_d \) and spin projection \( \sigma \). The hybridization between the \( d \)-electrons and the conduction electrons is characterized by the hybridization energy \( V_k \) and \( h \) is the Zeemann energy associated with an external magnetic field. Since we are only interested in the correlation functions of the impurity, we integrate over the conduction electrons using the functional integral representation of the model [7]. The generating functional \( G_{\beta}[J_d, J_c] \) of the connected Green’s functions can then be represented as the following ratio of the fermionic functional integrals:

\[
e^{G_{\beta}[J_d, J_c]} = \frac{\int \mathcal{D}[d, d] e^{-\mathcal{S}[\hat{d}_{\sigma}, \hat{d}_{\sigma}^\dagger] + (\hat{d}_{\sigma}, \hat{d}_{\sigma}^\dagger) + (\hat{d}_{\sigma}^\dagger, \hat{d}_{\sigma})} \int \mathcal{D}[d, d] e^{-\mathcal{S}[\hat{d}_{\sigma}, \hat{d}_{\sigma}^\dagger]}}{\int \mathcal{D}[d, d] e^{-\mathcal{S}[\hat{d}_{\sigma}, \hat{d}_{\sigma}^\dagger]}}. \quad (1.4)
\]

with the Euclidean action given by

\[
\mathcal{S}[\hat{d}_{\sigma}, \hat{d}_{\sigma}^\dagger] = \mathcal{S}_0[\hat{d}_{\sigma}, \hat{d}_{\sigma}^\dagger] + \mathcal{S}_V[\hat{d}_{\sigma}, \hat{d}_{\sigma}^\dagger] = -\int_0^\beta \sum_{\sigma} G^{-1}_{0,\sigma}(i\omega) \hat{d}_{\sigma\uparrow}^\dagger \hat{d}_{\sigma\uparrow} + U \int_0^\beta d\tau \hat{d}_{\uparrow}(\tau) \hat{d}_{\uparrow}(\tau) \hat{d}_{\downarrow}(\tau) \hat{d}_{\downarrow}(\tau). \quad (1.5)
\]
Here, \( \int_0^\beta \frac{1}{\beta} \sum_\omega \) denotes the summation over the fermionic Matsubara frequencies \( i\omega \) and \( \int_0^\beta d\tau \) denotes the integration over imaginary time, where \( \beta \) is the inverse temperature. The non-interacting Green’s function is

\[
G_{0,\sigma}(i\omega) = \frac{1}{i\omega - \xi_{0,\sigma} - \Delta_\sigma(i\omega)},
\]

where

\[
\xi_{0,\sigma} = E_d - \mu - \sigma \hbar
\]

is the energy of a localized \( d \)-electron with spin projection \( \sigma \) relative to the chemical potential \( \mu \), and the spin-dependent hybridization function is given by

\[
\Delta_\sigma(i\omega) = \sum_k \frac{|V_k|^2}{i\omega - \epsilon_k + \mu + \sigma \hbar}.
\]

The Fourier transform of the Grassmann fields \( d_\sigma(\tau) \) in frequency space is defined by

\[
d_\sigma(\tau) = \int_\omega e^{-i\omega \tau} d_{\omega\sigma}.
\]

The functional \( G_c[\bar{j}_\sigma, j_\sigma] \) in equation (1.4) depends on the Grassmann sources \( \bar{j}_\sigma \) and \( j_\sigma \), and we have introduced the following notation for the source terms:

\[
(\bar{j}, d) = \int_\omega \sum_\sigma \bar{j}_{\omega\sigma} d_{\omega\sigma}, \quad (d, j) = \int_\omega \sum_\sigma \bar{d}_{\omega\sigma} j_{\omega\sigma}.
\]

### 2. Functional Ward identities

#### 2.1. \( U(1) \) Ward identities due to the particle number and spin conservation in a magnetic field

The Euclidean action for the correlated impurity given in equation (1.5) is invariant under independent global \( U(1) \) transformations of the fields for a given spin projection. This symmetry implies that the generating functional \( G_c[\bar{j}_\sigma, j_\sigma] \) satisfies certain functional differential equations, so-called functional Ward identities. By taking functional derivatives of these relations, we derive the Yamada–Yosida identities for the self-energy. Following [1, 6], we perform a local gauge transformation on the fermion fields in the (imaginary) time domain

\[
d_\sigma(\tau) = e^{-i\alpha_\sigma(\tau)} d'_\sigma(\tau), \quad \bar{d}_\sigma(\tau) = e^{i\alpha_\sigma(\tau)} \bar{d}'_\sigma(\tau),
\]

where \( \alpha_\sigma(\tau) \) are arbitrary real functions. The interaction part \( S_I \) of our action \( S = S_0 + S_I \) is invariant under these transformations, so that

\[
S[e^{i\alpha_\sigma(\tau)} \bar{d}'_\sigma(\tau), e^{-i\alpha_\sigma(\tau)} d'_\sigma(\tau)] = S[\bar{d}_\sigma, d_\sigma] - i \int_0^\beta d\tau \sum_\sigma [\bar{d}'_\sigma(\tau) \partial_t \alpha_\sigma(\tau)] d'_\sigma(\tau)
\]

\[
+ i \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma \bar{d}'_\sigma(\tau)[\alpha_\sigma(\tau) - \alpha_\sigma(\tau')] \Delta_\sigma(\tau - \tau') d'_\sigma(\tau') + O(\alpha^2),
\]

where \( \Delta_\sigma(\tau) = \int_0^\omega e^{-i\omega \tau} \Delta_\sigma(i\omega) \). Using the invariance of the functional integral representation (1.4) of \( G_c[\bar{j}_\sigma, j_\sigma] \) with respect to a change of the integration variables \( d_\sigma \rightarrow d'_\sigma, \bar{d}_\sigma \rightarrow \bar{d}'_\sigma \) and expanding to linear order in the gauge factors \( \alpha_\sigma(\tau) \), we obtain the desired functional Ward...
identity [1, 6]. For our purpose, it is convenient to express the ‘current terms’ of this Ward identity via the generating functional $\Gamma[J_\sigma, j_\sigma]$ of the irreducible vertices, which is obtained from $G_\sigma[J_\sigma, j_\sigma]$ via a functional Legendre transformation [1, 6]:

$$\Gamma[J_\sigma, j_\sigma] = \langle \{ \bar{J}_\sigma(x) \} \rangle + \langle \{ \bar{j}_\sigma(x) \} \rangle - S_0[\bar{J}_\sigma, \bar{j}_\sigma],$$  \tag{2.3}

where on the right-hand side it is understood that the sources $\bar{J}_\sigma$ and $\bar{j}_\sigma$ should be calculated as the functions of the field averages $\bar{d}_\sigma$ and $\bar{d}_\sigma$ by solving the equations

$$\bar{d}_\sigma = \delta G_\sigma[J_\sigma, j_\sigma], \quad \bar{d}_\sigma = -\delta G_\sigma[J_\sigma, j_\sigma].$$  \tag{2.4}

After Fourier transformation to frequency space and some rearrangements analogous to those in [6, 8], we obtain the functional Ward identity

$$\int_{\omega'} \sum_{\sigma'} \left\{ \left( G_{0,\sigma'}^{-1}(i\omega' + i\bar{\omega}) - G_{0,\sigma'}^{-1}(i\omega') \right) \frac{\delta^2 G_c}{\delta f'_{\omega,\sigma'} \delta f'_{\omega,\sigma'}} + d_{\omega',\sigma'} \frac{\delta \Gamma}{\delta d_{\omega' + \bar{\omega},\sigma'}} - \bar{d}_{\omega' + \bar{\omega},\sigma'} \frac{\delta \Gamma}{\delta d_{\omega',\sigma'}} \right\} = 0,$$  \tag{2.5}

where $\bar{\omega}$ is an external bosonic Matsubara frequency. Summing both sides of this functional equation over $\sigma'$, we obtain the functional Ward identity due to the $U(1)$ symmetry associated with particle number conservation

$$\int_{\omega'} \sum_{\sigma'} \left\{ \left( G_{0,\sigma'}^{-1}(i\omega' + i\bar{\omega}) - G_{0,\sigma'}^{-1}(i\omega') \right) \frac{\delta^2 G_c}{\delta f'_{\omega,\sigma'} \delta f'_{\omega,\sigma'}} + d_{\omega',\sigma'} \frac{\delta \Gamma}{\delta d_{\omega' + \bar{\omega},\sigma'}} - \bar{d}_{\omega' + \bar{\omega},\sigma'} \frac{\delta \Gamma}{\delta d_{\omega',\sigma'}} \right\} = 0.$$  \tag{2.6}

To obtain the analogous $U(1)$ Ward identity associated with the conservation of the spin projection along the axis of the magnetic field, we multiply equation (2.5) by $\sigma'$ before summing over $\sigma'$, which yields

$$\int_{\omega'} \sum_{\sigma'} \sigma' \left\{ \left( G_{0,\sigma'}^{-1}(i\omega' + i\bar{\omega}) - G_{0,\sigma'}^{-1}(i\omega') \right) \frac{\delta^2 G_c}{\delta f'_{\omega,\sigma'} \delta f'_{\omega,\sigma'}} + d_{\omega',\sigma'} \frac{\delta \Gamma}{\delta d_{\omega' + \bar{\omega},\sigma'}} - \bar{d}_{\omega' + \bar{\omega},\sigma'} \frac{\delta \Gamma}{\delta d_{\omega',\sigma'}} \right\} = 0.$$  \tag{2.7}

2.2. SU (2) Ward identity due to spin conservation

In the absence of a magnetic field, our action (1.5) is invariant under arbitrary rotations in spin space. To derive the corresponding SU(2) Ward identity, we perform a local rotation in spin space,

$$\begin{pmatrix} d_1(t) \\ d_1(t) \end{pmatrix} = U(t) \begin{pmatrix} d_1'(t) \\ d_1'(t) \end{pmatrix},$$  \tag{2.8}

where the SU(2) matrix $U(t)$ can be written as

$$U(t) = e^{-i\omega \cdot \alpha(t)}.$$  \tag{2.9}

Here, $\sigma = [\sigma^1, \sigma^2, \sigma^3]$ is the vector of Pauli matrices and $\alpha(t)$ is a time-dependent three-component vector. Expanding to linear order in $\alpha(t)$ we obtain, after the same manipulations as in section 2.1, the following SU(2) Ward identity:

$$\int_{\omega'} \sum_{\sigma\sigma'} \sigma' \left\{ \left( G_0^{-1}(i\omega' + i\bar{\omega}) - G_0^{-1}(i\omega') \right) \frac{\delta^2 G_c}{\delta f'_{\omega,\sigma} \delta f'_{\omega,\sigma'}} + d_{\omega',\sigma'} \frac{\delta \Gamma}{\delta d_{\omega' + \bar{\omega},\sigma'}} - \bar{d}_{\omega' + \bar{\omega},\sigma'} \frac{\delta \Gamma}{\delta d_{\omega',\sigma'}} \right\} = 0.$$  \tag{2.10}
where the superscript $i = x, y, z$ labels the three components of the vector operator $\sigma$. Together with the particle number conservation Ward identity (2.6) these equations are equivalent to the four Ward identities

$$\int d\omega \left\{ \left[ G^{-1}_{0}(i\omega' + i\tilde{\omega}) - G^{-1}_{0}(i\omega') \right] \frac{\delta^2 G'}{\delta \bar{d}_{\omega+0} \delta \bar{d}_{\omega+0}} + \frac{\delta}{\delta \bar{d}_{\omega+0,\sigma}} - \frac{\delta}{\delta \bar{d}_{\omega+0,\sigma}} \delta^2 G' \right\} = 0,$$

(2.11)

where $\sigma, \sigma' \in \{\uparrow, \downarrow\}$ are now fixed spin projections. Note that in the absence of a magnetic field, the Green’s function and the self-energy are independent of the spin quantum number $\sigma$, so that we may write $G_{\sigma}(i\omega) = G(i\omega)$ and $\Sigma_{\sigma}(i\omega) = \Sigma(i\omega)$. For $i = z$, we have $\sigma_{\sigma'}^z = \sigma' b_{\sigma,\sigma'}$ so that equation (2.10) reduces to the zero-field limit of the $U(1)$ Ward identity (2.7) associated with the conservation of the spin component in the direction of the magnetic field.

### 3. Ward identities for the self-energy

#### 3.1. Particle number conservation

For the AIM in a magnetic field, the first terms in the functional Taylor expansion of the generating functional $\Gamma[\bar{d}_{\sigma}, d_{\sigma}]$ are of the form [6]

$$\Gamma[\bar{d}_{\sigma}, d_{\sigma}] = \Gamma_0 + \int d\omega \sum_{\sigma} \frac{\delta}{\delta \bar{d}_{\omega+0}} \int d\omega' \sum_{\sigma'} \frac{\delta}{\delta d_{\omega'+0}} \delta \bar{d}_{\omega+0} \delta d_{\omega'+0} + \frac{1}{2} \int d\omega \int d\omega' \int d\omega'' \int d\omega''' \frac{\delta^2}{\delta \bar{d}_{\omega} \delta \bar{d}_{\omega+0}} \delta d_{\omega+0} \delta d_{\omega+0} \delta d_{\omega+0} \delta d_{\omega+0}$$

$$\times U_{\omega,\omega'}^{(4)}(i\omega', i\omega'', i\omega, i\omega') \frac{\delta}{\delta \bar{d}_{\omega+0}} \frac{\delta}{\delta \bar{d}_{\omega+0}} \delta d_{\omega+0} \delta d_{\omega+0} + \mathcal{O}(\bar{d}^2 d^2),$$

(3.1)

where $\Gamma_0$ is proportional to the interaction correction to the grand canonical potential, $\Sigma_{\sigma}(i\omega)$ is the exact irreducible self-energy and $U_{\omega,\omega'}^{(4)}(i\omega', i\omega, i\omega')$ is the exact effective interaction. The term in the second line of our functional Ward identity (2.6) then yields

$$\int d\omega \sum_{\sigma} \left[ \frac{\delta}{\delta \bar{d}_{\omega+0}} \frac{\delta G}{\delta \bar{d}_{\omega+0}} \right] = \int d\omega \sum_{\sigma} \left[ \Sigma_{\sigma}(i\omega + i\tilde{\omega}) - \Sigma_{\sigma}(i\omega') \right] \bar{d}_{\omega+0} d_{\omega+0} + \mathcal{O}(\bar{d}^2 d^2),$$

(3.2)

To extract the Ward identity for the self-energy from our functional Ward identity (2.6), we take the second functional derivative $\frac{\delta^2}{\delta \bar{d}_{\omega} \delta d_{\omega'}}$ of both sides of equation (2.6) and then set all fields equal to zero, which yields

$$\Sigma_{\sigma}(i\omega + i\tilde{\omega}) = \Sigma_{\sigma}(i\omega) = -\int d\omega' \sum_{\sigma'} \left[ G^{-1}_{0,\sigma'}(i\omega' + i\tilde{\omega}) - G^{-1}_{0,\sigma'}(i\omega') \right]$$

$$\times G_{\sigma'}(i\omega' + i\tilde{\omega}) G_{\sigma'}(i\omega') U_{\omega,\omega'}^{(4)}(i\omega + i\tilde{\omega}, i\omega', i\omega' + i\tilde{\omega}, i\omega).$$

(3.3)

To obtain the right-hand side of this Ward identity, we have used

$$\frac{\delta}{\delta \bar{d}_{\omega}} \frac{\delta}{\delta d_{\omega'}} \frac{\delta^2 G}{\delta d_{\omega+0,\sigma}} \bigg|_{\text{fields}=0} = G_{\sigma}(i\omega') G_{\sigma}(i\omega' + i\tilde{\omega})$$

$$\times U_{\omega',\omega}^{(4)}(i\omega + i\tilde{\omega}, i\omega', i\omega' + i\tilde{\omega}, i\omega),$$

(3.4)

which follows from the tree expansion relating the connected Green’s functions generated by $G'$ to the irreducible vertices [6, 7]. In the limit of vanishing bosonic frequency $\tilde{\omega} \to 0$ the Ward identity (3.3) reduces to

$$\frac{\partial \Sigma_{\sigma}(i\omega)}{\partial (i\omega)} = -\int d\omega' \sum_{\sigma'} \left[ 1 - \frac{\partial}{\partial (i\omega')} \right] G^2_{\sigma'}(i\omega') G_{\sigma'}(i\omega', i\omega'),$$

(3.5)
where we have defined
\[ \Gamma_{\sigma,\sigma'}(i\omega, i\omega') = U_{\sigma,\sigma'}(i\omega, i\omega'; i\omega, i\omega). \] (3.6)

The above identities are valid for the arbitrary hybridization functions \( \Delta_\sigma(i\omega) \). Of special interest is the limit of the infinite bandwidth of the conduction electron band with flat density of states, where the general expression for \( \Delta_\sigma(i\omega) \) given in equation (1.8) is given by
\[ \Delta_\sigma(i\omega) = -i\Delta \text{sgn } \omega = -i\Delta[2\Theta(\omega) - 1]. \] (3.7)

Here, the hybridization energy \( \Delta \) is assumed to be independent of the chemical potential and the magnetic field. In this limit
\[ \frac{\partial \Delta_\sigma(i\omega')}{\partial (i\omega)} = -2\Delta \delta(i\omega'). \] (3.8)

The term \( \frac{\partial \Delta_\sigma(i\omega')}{\partial (i\omega')}G_{\sigma}^2(i\omega') \) in equation (3.5) is then ambiguous because the \( \delta \)-function in the first term is multiplied by the sign function associated with the hybridization function in \( G_{\sigma}^2(i\omega') \). To properly define this term, one should use the Morris lemma [9, 10], which states that the product of the delta-function with an arbitrary function \( f(\Theta(x)) \) of the \( \Theta - \text{function} \) should be defined via
\[ \delta(x)f(\Theta(x)) = \delta(x)\int_0^1 dt f(t). \] (3.9)

We conclude that in the infinite bandwidth limit
\[ -\frac{\partial \Delta_\sigma(i\omega')}{\partial (i\omega')}G_{\sigma}^2(i\omega') = 2\Delta \delta(i\omega')G_{\sigma}^2(i\omega') = 2\Delta \delta(i\omega')\int_0^1 dt \frac{1}{[-\xi_{\sigma'} + i\Delta(2t - 1)]^2} \]
\[ = \delta(i\omega') \frac{2\Delta}{\xi_{\sigma'}^2 + \Delta^2} \equiv 2\pi \delta(i\omega') \rho_{\sigma'}(0), \] (3.10)

where \( \xi_{\sigma} = \xi_{0,\sigma} + \Sigma_{\sigma}(i0) \) is the true excitation energy of a localized electron with spin projection \( \sigma \), and
\[ \rho_{\sigma}(0) = \frac{\Delta}{\pi} \frac{1}{\xi_{\sigma}^2 + \Delta^2} \] (3.11)
is the spectral density of the localized \( d \)-electron with spin \( \sigma \) at vanishing energy. Substituting equation (3.10) into (3.5) we obtain the corresponding Ward identity in the infinite bandwidth limit
\[ \frac{\partial \Sigma_{\sigma}(i\omega)}{\partial (i\omega)} = -\int_{i\omega} \sum_{\sigma'} G_{\sigma'}^2(i\omega')\Gamma_{\sigma,\sigma'}(i\omega, i\omega') - \sum_{\sigma'} \rho_{\sigma'}(0)\Gamma_{\sigma,\sigma'}(i\omega, 0). \] (3.12)

If we (incorrectly) replace \( \rho_{\sigma'}(0) \rightarrow \rho_{\sigma}(0) \) in the second line of equation (3.12), we arrive at equation (5.71) of [4].

Alternatively, we arrive at the Ward identity (3.12) without invoking the Morris lemma, if we choose the bosonic frequency \( \tilde{\omega} \) in equation (3.3) to be equal to \( 2\pi / \beta \), replace the integral \( \int_{i\omega} \) by the sum \( \sum_{n} \) with \( \omega_{\tilde{n}} = (2n + 1)\pi / \beta \), and finally take the limit \( \beta \rightarrow \infty \).

3.2. Spin conservation

The Ward identity for the self-energy associated with the conservation of the spin projection in the direction of the magnetic field can be derived analogously from the corresponding functional Ward identity (2.7). By comparing the functional Ward identity (2.7) due to particle number conservation with the corresponding $U(1)$ Ward identity (2.7) due to spin conservation, we conclude that in the spin case the Ward identities for the self-energy can be obtained from those of the particle number case by simply replacing

$$\sum_\sigma \rightarrow \sum_{\sigma'}.$$  \hspace{1cm} (3.14)

In particular, the spin analog of the particle number Ward identity (3.5) is

$$\sigma \frac{\partial \Sigma_{\sigma} (i\omega)}{\partial (i\omega)} = - \int \omega' \sum_{\sigma'} \sigma' \left[ 1 - \frac{\partial \Delta_{\sigma'} (i\omega')}{\partial (i\omega')} \right] G_{\sigma\sigma'}^2 (i\omega') \Gamma_{\sigma,\sigma'} (i\omega, i\omega').$$  \hspace{1cm} (3.15)

Combining this equation with the corresponding equation for the particle number, equation (3.5), we obtain the two Ward identities

$$\frac{\partial \Sigma_{\sigma} (i\omega)}{\partial (i\omega)} = - \int \omega' \left[ 1 - \frac{\partial \Delta_{\sigma} (i\omega')}{\partial (i\omega')} \right] G_{\sigma\sigma}^2 (i\omega') \Gamma_{\sigma,\sigma} (i\omega, i\omega'),$$  \hspace{1cm} (3.16)

$$0 = - \int \omega' \left[ 1 - \frac{\partial \Delta_{\sigma} (i\omega')}{\partial (i\omega')} \right] G_{\sigma\sigma'}^2 (i\omega') \Gamma_{\sigma,\sigma'} (i\omega, i\omega').$$  \hspace{1cm} (3.17)

In the limit of an infinite bandwidth, these equations can be written in analogy to equation (3.12) as

$$\frac{\partial \Sigma_{\sigma} (i\omega)}{\partial (i\omega)} = - \int \omega' G_{\sigma\sigma}^2 (i\omega') \Gamma_{\sigma,\sigma} (i\omega, i\omega') - \rho_\sigma (0) \Gamma_{\sigma,\sigma} (i\omega, 0),$$  \hspace{1cm} (3.18)

$$0 = - \int \omega' G_{\sigma\sigma'}^2 (i\omega') \Gamma_{\sigma,\sigma'} (i\omega, i\omega') - \rho_{-\sigma} (0) \Gamma_{\sigma,\sigma'} (i\omega, 0).$$  \hspace{1cm} (3.19)

Finally, we note that in the absence of a magnetic field the $SU(2)$ functional Ward identity (2.10) does not imply any further independent relation for the self-energy, since in this case we just have $\Sigma_{\sigma} (i\omega) = \Sigma(i\omega)$. However, taking higher order functional derivatives of equation (2.10), we may obtain symmetry relations involving higher order vertices, which are beyond the scope of this work.

4. Proof of the Yamada–Yosida identities

4.1. Relations between derivatives of the self-energy

The above Ward identities can now be used to derive exact relations between the derivatives of the self-energy with respect to frequency, chemical potential and magnetic field. In the book by Hewson [4], one can find a derivation of these identities using diagrammatic arguments. Here, we show that the correct relations can be obtained quite simply within the framework of the exact renormalization group (also known as the functional renormalization group) [5, 6]. As a special case of the general exact renormalization group equation for the irreducible
self-energy of an interacting Fermi system derived in [6, 11, 12], we find for the self-energy of the AIM

$$\partial_\Lambda \Sigma_\sigma (i\omega) = \int_{\omega'} \sum_{\sigma'} G_{\sigma'} (i\omega') \Gamma_{\sigma,\sigma'} (i\omega, i\omega'),$$

(4.1)

where we have used again the notation (3.6) for the effective interaction, and where \( \Lambda \) is some flow parameter (cutoff) appearing in the Gaussian part of the action. All Green’s functions and vertices in equation (4.1) implicitly depend on the parameter \( \Lambda \). The so-called single-scale propagator is defined by

$$G_\sigma (i\omega) = -G_\sigma^2 (i\omega) \partial_\Lambda G_{0,\sigma}^{-1} (i\omega).$$

(4.2)

The exact renormalization group flow equation (4.1) is valid for any choice of the flow parameter \( \Lambda \). In particular, we may choose the chemical potential \( \mu \) as a flow parameter [13]. Then, \( \Lambda = \mu \) and hence

$$\partial_\Lambda G_{0,\sigma}^{-1} (i\omega) = \frac{\partial}{\partial \mu} [i\omega - E_\mu + \mu + \sigma h - \Delta_\sigma (i\omega)]$$

$$= 1 - \frac{\partial \Delta_\sigma (i\omega)}{\partial \mu},$$

(4.3)

so that the single-scale propagator is simply

$$G_\sigma (i\omega) = -G_\sigma^2 (i\omega) \left[ 1 - \frac{\partial \Delta_\sigma (i\omega)}{\partial \mu} \right].$$

(4.4)

In this chemical potential cutoff scheme, the exact renormalization group flow equation (4.1) reduces to

$$\frac{\partial \Sigma_\sigma (i\omega)}{\partial \mu} = -\int_{\omega'} \sum_{\sigma'} \left[ 1 - \frac{\partial \Delta_{\sigma'} (i\omega')}{\partial \mu} \right] G_{\sigma'}^2 (i\omega') \Gamma_{\sigma',\sigma'} (i\omega, i\omega').$$

(4.5)

To further manipulate this expression, let us note that for \( \omega \neq 0 \), the integrand of the hybridization function given in equation (1.8) is non-singular, such that

$$\frac{\partial \Delta_\sigma (i\omega)}{\partial (i\omega)} = \frac{\partial \Delta_\sigma (i\omega)}{\partial \mu}, \quad \omega \neq 0. \quad (4.6)$$

For \( \omega = 0 \), however, we have to be more careful. Defining the spectral density

$$g (\epsilon) = \pi \sum_k |V_k|^2 \delta (\epsilon - \epsilon_k),$$

(4.7)

the hybridization function \( \Delta_\sigma (i\omega) \) can be rewritten as

$$\Delta_\sigma (i\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\epsilon g (\epsilon) \frac{1}{i\omega - \epsilon + \mu + \sigma h}.$$ \quad (4.8)

Using the well-known formula

$$\frac{1}{x \pm i0^+} = P \frac{1}{x} \mp i\pi \delta (x),$$

(4.9)

where \( P \) is the principle value, we see that \( \Delta_\sigma (\zeta) \) has a branch cut along the real axis. More explicitly, defining

$$\Delta = g (\mu + \sigma h),$$

(4.10)

we obtain

$$\frac{\partial \Delta_\sigma (i\omega)}{\partial (i\omega)} = \frac{\partial \Delta_\sigma (i\omega)}{\partial \mu} - 2\Delta \delta (\omega),$$

(4.11)
where the term $-2\Delta\delta(\omega)$ arises from the discontinuity across the branch cut. In the limit of a flat band of infinite width discussed above, $g(\epsilon) = \Delta$ for all $\epsilon$ and $\partial\Delta_\sigma(i\omega)/\partial\mu = 0$, so that equation (4.11) reduces to equation (3.8). Using identity (4.11) we may write our exact renormalization group flow equation (4.5) in the form

$$\frac{\partial \Sigma_\sigma(i\omega)}{\partial \mu} = -\int_\omega \sum_{\sigma'} \left[ 1 - \frac{\partial \Delta_\sigma(i\omega')}{\partial(i\omega')} - 2\Delta\delta(i\omega') \right] G_\sigma^2(i\omega') \Gamma_{\sigma,\sigma'}(i\omega, i\omega')$$

$$= -\int_\omega \sum_{\sigma'} \left[ 1 - \frac{\partial \Delta_\sigma(i\omega')}{\partial(i\omega')} \right] G_\sigma^2(i\omega') \Gamma_{\sigma,\sigma'}(i\omega, i\omega') + \sum_{\sigma'} \rho_{\sigma'}(0) \Gamma_{\sigma,\sigma'}(i\omega, 0).$$

(4.12)

Comparing the right-hand side of this exact relation with the right-hand side of the particle number Ward identity (3.5), we conclude that for all frequencies we have the following exact identity:

$$\frac{\partial \Sigma_\sigma(i\omega)}{\partial(i\omega)} = \frac{\partial \Sigma_\sigma(i\omega)}{\partial \mu} - \sum_{\sigma'} \rho_{\sigma'}(0) \Gamma_{\sigma,\sigma'}(i\omega, 0).$$

(4.13)

Next, let us choose in our exact renormalization group flow equation (4.1) the magnetic field as a flow parameter ($\Lambda = h$). The relevant single-scale propagator is then

$$G_\sigma(i\omega) = -G_\sigma^2(i\omega) \left[ \sigma - \frac{\partial \Delta_\sigma(i\omega)}{\partial h} \right].$$

(4.14)

and hence

$$\frac{\partial \Sigma_\sigma(i\omega)}{\partial h} = -\int_\omega \sum_{\sigma'} \left[ 1 - \sigma' \frac{\partial \Delta_\sigma(i\omega')}{\partial h} \right] G_\sigma^2(i\omega') \Gamma_{\sigma,\sigma'}(i\omega, i\omega').$$

(4.15)

Noting that

$$\frac{\Delta_\sigma(i\omega)}{\partial h} = \frac{\Delta_\sigma(i\omega)}{\partial \mu},$$

(4.16)
equation (4.15) can also be written as

$$\frac{\partial \Sigma_\sigma(i\omega)}{\partial h} = -\int_\omega \sum_{\sigma'} \left[ 1 - \frac{\partial \Delta_\sigma(i\omega')}{\partial(i\omega')} - 2\Delta\delta(i\omega') \right] G_\sigma^2(i\omega') \Gamma_{\sigma,\sigma'}(i\omega, i\omega')$$

$$= -\int_\omega \sum_{\sigma'} \left[ 1 - \frac{\partial \Delta_\sigma(i\omega')}{\partial(i\omega')} \right] G_\sigma^2(i\omega') \Gamma_{\sigma,\sigma'}(i\omega, i\omega') + \sum_{\sigma'} \sigma' \rho_{\sigma'}(0) \Gamma_{\sigma,\sigma'}(i\omega, 0).$$

(4.17)

Comparing this with the $U(1)$ spin Ward identity (3.15), we conclude that

$$\frac{\partial \Sigma_\sigma(i\omega)}{\partial(i\omega)} = \sigma - \frac{\partial \Sigma_\sigma(i\omega)}{\partial h} - \sigma \sum_{\sigma'} \sigma' \rho_{\sigma'}(0) \Gamma_{\sigma,\sigma'}(i\omega, 0).$$

(4.18)

Of particular interest are the above relations for $\omega \to 0$, because in this limit the $\omega$-derivative determines the wavefunction renormalization factor $Z_\sigma$ via

$$\frac{\partial \Sigma_\sigma(i\omega)}{\partial(i\omega)} \bigg|_{\omega=0} = 1 - Z_\sigma^{-1}.$$  

(4.19)

Taking the limit $\omega \to 0$ in equations (4.13) and (4.18) and using the fact that due to antisymmetry the effective interaction at vanishing frequencies has the form

$$U_{\sigma,\sigma'}^{(i)}(0, 0; 0, 0) = \Gamma_{\sigma,\sigma'}(0, 0) = \delta_{\sigma,\sigma'} \Gamma_{\sigma,\sigma},$$

(4.20)
we obtain
\[
\begin{align*}
\frac{\partial \Sigma_\sigma (i\omega)}{\partial (i\omega)} \bigg|_{i\omega=0} &= \frac{\partial \Sigma_\sigma (0)}{\partial \mu} - \rho_{-\sigma} (0) \Gamma_{\sigma,-\sigma}, \\
\frac{\partial \Sigma_\sigma (i\omega)}{\partial (i\omega)} \bigg|_{i\omega=0} &= \frac{\partial \Sigma_\sigma (0)}{\partial \mu} + \rho_{-\sigma} (0) \Gamma_{\sigma,-\sigma}.
\end{align*}
\] (4.21)

(4.22)

Adding and subtracting these equations, we obtain
\[
\begin{align*}
2 \frac{\partial \Sigma_\sigma (i\omega)}{\partial (i\omega)} \bigg|_{i\omega=0} &= \frac{\partial \Sigma_\sigma (0)}{\partial \mu} + \rho_{\sigma} (0) \frac{\partial \Sigma_\sigma (0)}{\partial \mu}, \\
2 \rho_{-\sigma} (0) \Gamma_{\sigma,-\sigma} &= \frac{\partial \Sigma_\sigma (0)}{\partial \mu} - \rho_{\sigma} (0) \frac{\partial \Sigma_\sigma (0)}{\partial \mu}.
\end{align*}
\] (4.23)

(4.24)

Equation (4.23) is a corrected version of equation (5.80) of [4].

4.2. Yamada–Yosida identities

To make contact with the work of Yamada and Yosida [2], we now assume a flat density of states and take the limit of an infinite width of the conduction electron band, \(D \to \infty\). Then there is a simple exact relation between the occupation numbers \(n_\sigma\) of the impurity level and the self-energies \(\Sigma_\sigma (i0)\) at vanishing frequency [4]:
\[
n_\sigma = \frac{1}{2} \left( 1 - \frac{1}{\pi} \arctan \left[ \frac{E_{\sigma} - \mu - \sigma h + \Sigma_\sigma (i0)}{\Delta} \right] \right). 
\] (4.25)

Taking derivatives of this expression with respect to \(\mu\) and \(h\), we obtain
\[
\begin{align*}
\frac{\partial n_\sigma}{\partial \mu} &= \rho_\sigma (0) \left[ 1 - \frac{\partial \Sigma_\sigma (i0)}{\partial \mu} \right], \\
\sigma \frac{\partial n_\sigma}{\partial h} &= \rho_\sigma (0) \left[ 1 - \sigma \frac{\partial \Sigma_\sigma (i0)}{\partial h} \right].
\end{align*}
\] (4.26)

(4.27)

Hence,
\[
\begin{align*}
\frac{\partial \Sigma_\sigma (i0)}{\partial \mu} &= 1 - \frac{1}{\rho_\sigma (0)} \frac{\partial n_\sigma}{\partial \mu}, \\
\sigma \frac{\partial \Sigma_\sigma (i0)}{\partial h} &= 1 - \frac{1}{\rho_\sigma (0)} \sigma \frac{\partial n_\sigma}{\partial h}.
\end{align*}
\] (4.28)

(4.29)

Substituting these relations into the Ward identities (4.23) and (4.24), we obtain for the \(\omega\)-derivative of the self-energy
\[
\frac{\partial \Sigma_\sigma (i\omega)}{\partial (i\omega)} \bigg|_{i\omega=0} = 1 - \frac{1}{2 \rho_\sigma (0)} \left[ \frac{\partial n_\sigma}{\partial \mu} + \sigma \frac{\partial n_\sigma}{\partial h} \right], 
\] (4.30)

and for the effective interaction at zero energy
\[
\Gamma_{\sigma,-\sigma} = -\frac{1}{2 \rho_{\sigma} (0) \rho_{-\sigma} (0)} \left[ \frac{\partial n_\sigma}{\partial \mu} - \sigma \frac{\partial n_\sigma}{\partial h} \right].
\] (4.31)

For \(h \to 0\), the self-energy and the density of states are independent of the spin projection, so that we may write \(\Sigma_\sigma (i\omega) = \Sigma (i\omega), \rho_{\sigma} (0) = \rho (0)\) and \(\Gamma_{\sigma,-\sigma} = \Gamma_{\perp}\). As in [2], we now
focus on the particle–hole symmetric case, where \( \rho(0) = 1/(\pi \Delta) \) in the flat band infinite bandwidth limit considered here. Averaging both sides of equations (4.30) and (4.31) over both spin projections, we obtain the Ward identities

\[
\frac{\partial \Sigma_\sigma (i\omega)}{\partial (i\omega)} \bigg|_{\omega=0} = 1 - \frac{\tilde{\chi}_c + \tilde{\chi}_s}{2},
\]

(4.32)

\[
\rho(0) \Gamma_\perp = -\frac{\tilde{\chi}_c - \tilde{\chi}_s}{2},
\]

(4.33)

where the dimensionless particle number (charge) and spin susceptibilities are defined by

\[
\tilde{\chi}_c = \frac{\chi_c}{\rho(0)} = \frac{\pi}{\Delta^2} \sum_\sigma \frac{\partial n_\sigma}{\partial \mu},
\]

(4.34)

\[
\tilde{\chi}_s = \frac{\chi_s}{\rho(0)} = \frac{\pi}{\Delta^2} \sum_\sigma \frac{\partial n_\sigma}{\partial \hbar},
\]

(4.35)

Identities (4.32) and (4.33) have first been obtained by Yamada and Yosida [2], who showed that both sides of these equations have identical series expansions in powers of \( U/\Delta \). Such a perturbative proof relies on the assumption that there are no non-analytic terms which are missed by the series expansions. Our proof of equations (4.32) and (4.33) given above shows more clearly that these identities are a direct consequence of the \( U(1) \times U(1) \) symmetry associated with the particle number and spin conservation of the AIM in a magnetic field. Moreover, our derivation of equations (4.32) and (4.33) is non-perturbative, because it relies only on the symmetries of the AIM and the associated functional Ward identities and on the exact renormalization group flow equation for the irreducible self-energy.

Using relation (4.19), we see that identity (4.32) implies that the wavefunction renormalization factor of the AIM can be expressed in terms of the susceptibilities as

\[
Z = \frac{2}{\tilde{\chi}_c + \tilde{\chi}_s}.
\]

(4.36)

The other Ward identity (4.33) allows us to express the imaginary part of the retarded self-energy to the susceptibilities. Therefore, we recall that the skeleton equation for the self-energy of the AIM (which is a consequence of the Dyson–Schwinger equation, which in turn follows within a functional integral approach from the invariance of the functional integral under infinitesimal shifts of the fields [1, 6]) implies the following exact expression for the imaginary part of the self-energy of the symmetric AIM in the infinite bandwidth limit [4]:

\[
\text{Im} \Sigma(\omega + i0) = -\left( \frac{\Gamma_\perp}{\pi \Delta} \right)^2 \frac{\omega^2}{2\Delta} + O(\omega^3).
\]

(4.37)

Substituting identity (4.33) for the dimensionless effective interaction \( \Gamma_\perp/(\pi \Delta) = \rho(0) \Gamma_\perp \), we obtain

\[
\text{Im} \Sigma(\omega + i0) = -\left( \frac{\tilde{\chi}_c - \tilde{\chi}_s}{2} \right)^2 \frac{\omega^2}{2\Delta} + O(\omega^3).
\]

(4.38)

On the imaginary frequency axis, the low-frequency expansion of the self-energy of the symmetric AIM in the infinite bandwidth limit is therefore

\[
\Sigma(i\omega) = \frac{U}{2} + \left( 1 - \frac{\tilde{\chi}_c + \tilde{\chi}_s}{2} \right) i\omega + i\left( \frac{\tilde{\chi}_c - \tilde{\chi}_s}{8\Delta} \right) \omega^2 \text{ sgn } \omega + \text{analytic terms } O(\omega^3).
\]

(4.39)
Taking the different notations for the dimensionless susceptibilities into account\textsuperscript{5}, equation (4.39) agrees with the expressions derived by Yamada and Yosida [2].

5. Conclusions

In this work, we have used modern functional methods to give a non-perturbative proof of the Yamada--Yosida identities, which express the coefficients in the low-frequency expansion of the self-energy of the AIM in terms of thermodynamic susceptibilities. In contrast to the derivation of these relations given by Yamada and Yosida [2], which is based on a series expansion in powers of the interaction, our non-perturbative proof relies on exact Ward identities and on an exact renormalization group flow equation for the irreducible self-energy. From our derivation, it is obvious that the Yamada--Yosida identities are a direct consequence of the $U(1) \times U(1)$ symmetry of the AIM associated with the conservation of the particle number and the total spin component in the direction of an external magnetic field.

We have also presented a thorough derivation of the general functional Ward identities of the AIM due to the particle number and spin conservation. Furthermore, we have shown that various identities relating the derivatives of the self-energy with respect to frequency, chemical potential and magnetic field can be obtained by combining the Ward identities with exact renormalization group flow equations for the self-energy.

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\textsuperscript{5} Our dimensionless particle number (charge) and spin susceptibilities $\tilde{\chi}_c$ and $\tilde{\chi}_s$ are related to the quantities $\tilde{\chi}_{\text{even}} = \tilde{\chi}_{\uparrow\uparrow}$ and $\tilde{\chi}_{\text{odd}} = \tilde{\chi}_{\uparrow\downarrow}$ introduced by Yamada and Yosida [2] and by Oguri [3] via $\tilde{\chi}_c = \tilde{\chi}_{\text{even}} + \tilde{\chi}_{\text{odd}}$ and $\tilde{\chi}_s = \tilde{\chi}_{\text{even}} - \tilde{\chi}_{\text{odd}}$, so that $(\tilde{\chi}_c + \tilde{\chi}_s)/2 = \tilde{\chi}_{\text{even}} = \tilde{\chi}_{\uparrow\uparrow}$ and $(\tilde{\chi}_c - \tilde{\chi}_s)/2 = \tilde{\chi}_{\text{odd}} = \tilde{\chi}_{\uparrow\downarrow}$.