Functional renormalization group without functional integrals: implementing Hilbert space projections for strongly correlated electrons via Hubbard X-operators

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Exact functional renormalization group (FRG) flow equations for quantum systems can be derived directly within an operator formalism without using functional integrals. This simple insight opens new possibilities for applying FRG methods to models for strongly correlated electrons with projected Hilbert spaces, such as quantum spin models, the t-J model, or the Hubbard model at infinite on-site repulsion. By representing these models in terms of Hubbard X-operators, we derive exact flow equations for the time-ordered correlation functions of the X-operators (X-FRG), which allow us to calculate the electronic correlation functions in the projected Hilbert space of these models. The Hubbard-I approximation for the single-particle Green function of the Hubbard model is recovered from a trivial truncation of the flow equations where the two-point vertex is approximated by its atomic limit. We use our approach to calculate the quasi-particle residue and damping in the "hidden Fermi liquid" state of the Hubbard model at infinite on-site repulsion where the Hamiltonian consists only of the projected kinetic energy.

I. INTRODUCTION

The functional renormalization group (FRG) has been used by a growing number of researchers to study a variety of problems in field theory and statistical physics, ranging from classical and quantum critical phenomena over correlated lattice models for interacting fermions or bosons, to quantum chromodynamics and quantum gravity, see Refs. 11-5 for reviews. Usually, derivations of FRG flow equations use functional integral representations of suitably defined generating functionals 11-6. However, functional integrals are really not necessary for the derivation of FRG flow equations for quantum systems 2, 7. It seems that this simple insight has not been sufficiently appreciated by researchers working in the field. In this work we will show how to derive FRG flow equations for quantum systems directly within a Hamiltonian formalism, avoiding the representation of correlation functions in terms of functional integrals. This should be helpful for teaching FRG methods to students who are not familiar with functional integrals. More importantly, this insight leads to new possibilities of applying FRG methods to quantum systems with projected Hilbert spaces or to systems whose Hamiltonian is defined in terms of a set of operators satisfying noncanonical commutation relations. An important example are quantum spin systems for which exact flow equations for the spin correlation functions can be derived directly from the representation of the corresponding generating functional as a time-ordered exponential 7. Recent applications of our spin-FRG approach can be found in Refs. 7-14.

In this work we will show that this strategy can also be used to derive formally exact FRG flow equations for fermionic lattice models with projected Hilbert spaces such as the t-J model or the Hubbard model with infinitely strong on-site repulsion. Therefore, we express these models in terms of so-called Hubbard X-operators

[15] 17] which satisfy non-canonical commutation relations. For the *t-J* model, this representation is convenient to implement the exclusion of states with doubly occupied lattice sites from the relevant Hilbert space. For the Hubbard model, this offers a non-perturbative route to study the physics at strong coupling [15]. Our X-FRG approach generalizes the spin-FRG [7]-14] to fermionic lattice models and is based on the observation that within a Hamiltonian formalism we can derive exact flow equations for generating functionals even if the Hamiltonian is expressed in terms of operators satisfying non-canonical commutation relations.

The rest of this work is organized as follows: In Sec. II we show how the Wetterich equation 6 for canonical fermions and bosons can be derived without using functional integrals. Our spin-FRG approach 7-14 and its extension to strongly correlated electronic systems using Hubbard X-operators presented in this work relies on a similar strategy. In Sec. III we define the Hubbard X-operators 15-17 and express the Hubbard and t-Jmodels in terms of these operators. In Sec. IV we use the method outlined in Sec. II to derive formally exact generalized Wetterich equations for the Hubbard and the t-J models in X-operator representation. In Sec. \overline{V} we present the first two applications of our method: First of all, we show how the so-called Hubbard-I approximation for the single-particle Green function of the Hubbard model emerges from the simplest possible truncation of our X-FRG flow equations. Moreover, from a level-1 truncation of the X-FRG flow equations, where the fourpoint vertex is approximated by its initial value corresponding to vanishing hopping, we calculate the quasiparticle residue and the quasi-particle damping of the Hubbard model at infinite on-site repulsion. Finally, in Sec. VI we summarize our results and point out possible future applications of our method. In three appendices, we present technical details of the calculation of timeordered correlation functions of the X-operators in the

atomic Hubbard model, where the hopping is switched off and the lattice sites are decoupled.

II. FRG WITHOUT FUNCTIONAL INTEGRALS

Before formulating the X-FRG approach, let us carefully explain why functional integrals are not necessary for the derivation of exact FRG flow equations for canonical bosons or fermions. In this section, we therefore consider a general second-quantized Hamiltonian of a bosonic or fermionic many-body system,

$$\mathcal{H} = \sum_{\mathbf{k}} \epsilon(\mathbf{k}) a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \mathcal{H}_{\text{int}}, \qquad (2.1)$$

where $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^{\dagger}$ are canonical bosonic or fermionic annihilation and creation operators, and \mathcal{H}_{int} is an arbitrary many-body interaction. The generating functional $\mathcal{G}[\bar{j},j]$ of the connected imaginary-time ordered correlation functions is defined in terms of the following trace of a time-ordered exponential over Fock space:

$$e^{\mathcal{G}[\bar{j},j]} = \operatorname{Tr}\left\{e^{-\beta\tilde{\mathcal{H}}}\mathcal{T}e^{\int_0^\beta d\tau \sum_{\mathbf{k}} \left[\bar{j}_{\mathbf{k}}(\tau) a_{\mathbf{k}}^\dagger(\tau) + a_{\mathbf{k}}^\dagger(\tau) j_{\mathbf{k}}(\tau)\right]}\right\},$$
(2.2)

where $\beta = 1/T$ is the inverse temperature and \mathcal{T} represents time-ordering in imaginary time. The sources $j_{\mathbf{k}}(\tau)$ and $\bar{j}_{\mathbf{k}}(\tau)$ are complex numbers for bosons and Grassmann variables for fermions, and

$$\tilde{\mathcal{H}} = \mathcal{H} - \mu \sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} = \sum_{\mathbf{k}} \left[\epsilon(\mathbf{k}) - \mu \right] a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \mathcal{H}_{\text{int}} \quad (2.3)$$

is the grand canonical Hamiltonian, where μ is the chemical potential. The time evolution of the operators $a_{\pmb k}(\tau)$ and $a^\dagger_{\pmb k}(\tau)$ is in the imaginary time Heisenberg picture, i.e., $a_{\pmb k}(\tau)=e^{\tilde{\mathcal H}\tau}a_{\pmb k}e^{-\tilde{\mathcal H}\tau}$ and $a^\dagger_{\pmb k}(\tau)=e^{\tilde{\mathcal H}\tau}a^\dagger_{\pmb k}e^{-\tilde{\mathcal H}\tau}.$ For our purpose, it is more convenient to rewrite the

For our purpose, it is more convenient to rewrite the generating functional (2.2) in the interaction picture (18). Therefore, we express our grand canonical Hamiltonian $\tilde{\mathcal{H}}$ as a sum of two terms:

$$\tilde{\mathcal{H}} = \mathcal{H}_1 + \mathcal{H}_2. \tag{2.4}$$

This decomposition is not unique and below we will use this freedom to derive FRG flow equations. In the interaction picture with respect to \mathcal{H}_1 the generating functional (2.2) can then be written as

$$e^{\mathcal{G}[\bar{j},j]} = \operatorname{Tr} \left\{ e^{-\beta \mathcal{H}_1} \mathcal{T} \left[e^{-\int_0^\beta d\tau \mathcal{H}_2(\tau)} \right] \times e^{\int_0^\beta d\tau \sum_{\mathbf{k}} \left[\bar{j}_{\mathbf{k}}(\tau) a_{\mathbf{k}}(\tau) + a_{\mathbf{k}}^{\dagger}(\tau) j_{\mathbf{k}}(\tau) \right]} \right] \right\}, \quad (2.5)$$

where now the time-dependence of all operators on the

right-hand side is generated by \mathcal{H}_1 , i.e.,

$$\mathcal{H}_2(\tau) = e^{\mathcal{H}_1 \tau} \mathcal{H}_2 e^{-\mathcal{H}_1 \tau}, \tag{2.6a}$$

$$a_{\mathbf{k}}(\tau) = e^{\mathcal{H}_1 \tau} a_{\mathbf{k}} e^{-\mathcal{H}_1 \tau}, \qquad (2.6b)$$

$$a_{\mathbf{k}}^{\dagger}(\tau) = e^{\mathcal{H}_1 \tau} a_{\mathbf{k}}^{\dagger} e^{-\mathcal{H}_1 \tau}.$$
 (2.6c)

By taking derivatives of the right-hand side of Eq. (2.5) with respect to the sources $j_{\mathbf{k}}(\tau)$ and $\bar{j}_{\mathbf{k}}(\tau)$ and subsequently setting the sources equal to zero, we generate the usual expressions for the imaginary-time ordered connected correlation functions in the interaction picture.

To derive formally exact FRG flow equations, we add a scale-dependent regulator to our Hamiltonian,

$$\tilde{\mathcal{H}}_{\Lambda} = \tilde{\mathcal{H}} + \sum_{\mathbf{k}} R_{\Lambda}(\mathbf{k}) a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}
= \sum_{\mathbf{k}} \left[\epsilon(\mathbf{k}) - \mu + R_{\Lambda}(\mathbf{k}) \right] a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \mathcal{H}_{\text{int}}.$$
(2.7)

The regulator $R_{\Lambda}(\mathbf{k})$ depends on a continuous scale parameter Λ . It is chosen such that at the initial scale $\Lambda = \Lambda_0$ the model can be solved in a controlled way, while at the final scale $\Lambda = \Lambda_1$ the regulator vanishes, $R_{\Lambda=\Lambda_1}(\mathbf{k})=0$, so that the original system is recovered. Using the interaction representation (2.5) with $\mathcal{H}_1=\mathcal{H}_{\rm int}$ and $\mathcal{H}_2=\sum_{\mathbf{k}}[\epsilon(\mathbf{k})-\mu+R_{\Lambda}(\mathbf{k})]a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}$ we obtain the following representation of the scale-dependent generating functional $\mathcal{G}_{\Lambda}[\bar{j},j]$ of the connected correlation functions of our deformed theory,

$$e^{\mathcal{G}_{\Lambda}[\bar{j},j]} = \text{Tr} \left\{ e^{-\beta \mathcal{H}_{\text{int}}} \mathcal{T} \left[e^{-\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} [\epsilon(\mathbf{k}) - \mu + R_{\Lambda}(\mathbf{k})] a_{\mathbf{k}}^{\dagger}(\tau) a_{\mathbf{k}}(\tau)} \right] \times e^{\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\bar{j}_{\mathbf{k}}(\tau) a_{\mathbf{k}}(\tau) + a_{\mathbf{k}}^{\dagger}(\tau) j_{\mathbf{k}}(\tau) \right]} \right] \right\}. \quad (2.8)$$

Alternatively, we may choose $\mathcal{H}_1 = \tilde{\mathcal{H}}$ and $\mathcal{H}_2 = \sum_{\mathbf{k}} R_{\Lambda}(\mathbf{k}) a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}$, which yields

$$e^{\mathcal{G}_{\Lambda}[\bar{j},j]} = \text{Tr} \left\{ e^{-\beta \tilde{\mathcal{H}}} \mathcal{T} \left[e^{-\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} R_{\Lambda}(\mathbf{k}) a_{\mathbf{k}}^{\dagger}(\tau) a_{\mathbf{k}}(\tau)} \right. \right. \\ \left. \times e^{\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\bar{j}_{\mathbf{k}}(\tau) a_{\mathbf{k}}(\tau) + a_{\mathbf{k}}^{\dagger}(\tau) j_{\mathbf{k}}(\tau) \right]} \right] \right\}, \quad (2.9)$$

where the time-dependence is in the Heisenberg picture with respect to the regulator-independent Hamiltonian $\tilde{\mathcal{H}}$. Using either Eq. (2.8) or (2.9), we may take the derivative with respect to Λ of both sides and represent the operators $a_{\mathbf{k}}(\tau)$ and $a_{\mathbf{k}}^{\dagger}(\tau)$ in the time-ordered expectation value as derivatives with respect to the sources, which can then be pulled out of the time-ordering bracket. Explicitly, for the representation (2.9) the chain of identities is

$$e^{\mathcal{G}_{\Lambda}[\bar{j},j]}\partial_{\Lambda}\mathcal{G}_{\Lambda}[\bar{j},j] = -\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\partial_{\Lambda}R_{\Lambda}(\mathbf{k})\right] \operatorname{Tr} \left\{ e^{-\beta\tilde{\mathcal{H}}}\mathcal{T} \left[e^{-\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} R_{\Lambda}(\mathbf{k})a_{\mathbf{k}}^{\dagger}(\tau)a_{\mathbf{k}}(\tau)} \right] \right\}$$

$$\times a_{\mathbf{k}}^{\dagger}(\tau)a_{\mathbf{k}}(\tau)e^{\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\bar{j}_{\mathbf{k}}(\tau)a_{\mathbf{k}}(\tau) + a_{\mathbf{k}}^{\dagger}(\tau)j_{\mathbf{k}}(\tau)\right] \right] \right\}$$

$$= -\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\partial_{\Lambda}R_{\Lambda}(\mathbf{k}) \right] \operatorname{Tr} \left\{ e^{-\beta\tilde{\mathcal{H}}}\mathcal{T} \left[e^{-\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} R_{\Lambda}(\mathbf{k})a_{\mathbf{k}}^{\dagger}(\tau)a_{\mathbf{k}}(\tau)} \right] \right\}$$

$$\times \zeta \frac{\delta}{\delta j_{\mathbf{k}}(\tau)} \frac{\delta}{\delta \bar{j}_{\mathbf{k}}(\tau)} e^{\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\bar{j}_{\mathbf{k}}(\tau)a_{\mathbf{k}}(\tau) + a_{\mathbf{k}}^{\dagger}(\tau)j_{\mathbf{k}}(\tau) \right]} \right\}$$

$$= -\zeta \int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\partial_{\Lambda}R_{\Lambda}(\mathbf{k}) \right] \frac{\delta}{\delta j_{\mathbf{k}}(\tau)} \frac{\delta}{\delta \bar{j}_{\mathbf{k}}(\tau)} \operatorname{Tr} \left\{ e^{-\beta\tilde{\mathcal{H}}}\mathcal{T} \left[e^{-\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} R_{\Lambda}(\mathbf{k})a_{\mathbf{k}}^{\dagger}(\tau)a_{\mathbf{k}}(\tau)} \right] \right\}$$

$$= -\zeta \int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\partial_{\Lambda}R_{\Lambda}(\mathbf{k}) \right] \frac{\delta}{\delta j_{\mathbf{k}}(\tau)} \frac{\delta}{\delta \bar{j}_{\mathbf{k}}(\tau)} \operatorname{Tr} \left\{ e^{-\beta\tilde{\mathcal{H}}}\mathcal{T} \left[e^{-\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} R_{\Lambda}(\mathbf{k})a_{\mathbf{k}}^{\dagger}(\tau)a_{\mathbf{k}}(\tau)} \right] \right\}$$

$$= -\zeta \int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\partial_{\Lambda}R_{\Lambda}(\mathbf{k}) \right] \frac{\delta}{\delta j_{\mathbf{k}}(\tau)} \frac{\delta}{\delta \bar{j}_{\mathbf{k}}(\tau)} \operatorname{Tr} \left\{ e^{-\beta\tilde{\mathcal{H}}}\mathcal{T} \left[e^{-\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} R_{\Lambda}(\mathbf{k})a_{\mathbf{k}}^{\dagger}(\tau)a_{\mathbf{k}}(\tau)} \right] \right\}$$

$$= -\zeta \int_{0}^{\infty} d\tau \sum_{\mathbf{k}} \left[\partial_{\Lambda} \mathbf{R}_{\Lambda}(\mathbf{k}) \right] \frac{1}{\delta j_{\mathbf{k}}(\tau)} \frac{1}{\delta \bar{j}_{\mathbf{k}}(\tau)} \left\{ e^{-\gamma \int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\bar{j}_{\mathbf{k}}(\tau) a_{\mathbf{k}}(\tau) + a_{\mathbf{k}}^{\dagger}(\tau) j_{\mathbf{k}}(\tau) \right]} \right\}$$

$$\times e^{\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\bar{j}_{\mathbf{k}}(\tau) a_{\mathbf{k}}(\tau) + a_{\mathbf{k}}^{\dagger}(\tau) j_{\mathbf{k}}(\tau) \right]} \right\}$$

$$(2.10c)$$

$$= -\zeta \int_{0}^{\beta} d\tau \sum \left[\partial_{\Lambda} R_{\Lambda}(\mathbf{k})\right] \frac{\delta}{\delta j_{\mathbf{k}}(\tau)} \frac{\delta}{\delta \bar{j}_{\mathbf{k}}(\tau)} e^{\mathcal{G}_{\Lambda}[\bar{j},j]}, \tag{2.10d}$$

where $\zeta = 1$ for bosons and $\zeta = -1$ for fermions. Carrying out the functional derivatives, we obtain the following exact flow equation for the generating functional of connected correlation functions:

$$\partial_{\Lambda} \mathcal{G}_{\Lambda}[\bar{j},j] = -\zeta \int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\partial_{\Lambda} R_{\Lambda}(\mathbf{k}) \right] \left\{ \frac{\delta^{2} \mathcal{G}_{\Lambda}[\bar{j},j]}{\delta j_{\mathbf{k}}(\tau) \delta \bar{j}_{\mathbf{k}}(\tau)} + \frac{\delta \mathcal{G}_{\Lambda}[\bar{j},j]}{\delta j_{\mathbf{k}}(\tau)} \frac{\delta \mathcal{G}_{\Lambda}[\bar{j},j]}{\delta \bar{j}_{\mathbf{k}}(\tau)} \right\}. \tag{2.11}$$

The fermionic version $(\zeta = -1)$ of this flow equation has already been derived in Ref. 8. To derive the corresponding Wetterich equation 3.6.8, we introduce the generating functional of the cutoff-dependent irreducible vertices via the usual subtracted Legendre transformation,

$$\Gamma_{\Lambda}[\bar{\psi},\psi] = \int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\bar{j}_{\mathbf{k}}(\tau) \psi_{\mathbf{k}}(\tau) + \bar{\psi}_{\mathbf{k}}(\tau) j_{\mathbf{k}}(\tau) \right] - \mathcal{G}_{\Lambda}[\bar{j},j] - \int_{0}^{\beta} d\tau \sum_{\mathbf{k}} R_{\Lambda}(\mathbf{k}) \bar{\psi}_{\mathbf{k}}(\tau) \psi_{\mathbf{k}}(\tau), \tag{2.12}$$

where on the right-hand side the sources \bar{j} and j should be expressed in terms of the operator expectation values ψ and $\bar{\psi}$ by inverting the relations

$$\psi_{\mathbf{k}}(\tau) = \langle \mathcal{T} a_{\mathbf{k}}(\tau) \rangle = \frac{\delta \mathcal{G}_{\Lambda}[\bar{j}, j]}{\delta \bar{j}_{\mathbf{k}}(\tau)}, \qquad \bar{\psi}_{\mathbf{k}}(\tau) = \langle \mathcal{T} a_{\mathbf{k}}^{\dagger}(\tau) \rangle = \zeta \frac{\delta \mathcal{G}_{\Lambda}[\bar{j}, j]}{\delta j_{\mathbf{k}}(\tau)}. \tag{2.13}$$

Here, the symbol $\langle \mathcal{T}A(\tau) \rangle$ denotes the time-ordered expectation value in the presence of sources, i.e.,

$$\langle \mathcal{T}A(\tau) \rangle = \frac{\text{Tr} \left\{ e^{-\beta \tilde{\mathcal{H}}} \mathcal{T} \left[A(\tau) e^{-\int_0^\beta d\tau \sum_{\mathbf{k}} R_{\Lambda}(\mathbf{k}) a_{\mathbf{k}}^{\dagger}(\tau) a_{\mathbf{k}}(\tau)} e^{\int_0^\beta d\tau \sum_{\mathbf{k}} \left[\bar{\jmath}_{\mathbf{k}}(\tau) a_{\mathbf{k}}(\tau) + a_{\mathbf{k}}^{\dagger}(\tau) j_{\mathbf{k}}(\tau) \right] \right] \right\}}{\text{Tr} \left\{ e^{-\beta \tilde{\mathcal{H}}} \mathcal{T} \left[e^{-\int_0^\beta d\tau \sum_{\mathbf{k}} R_{\Lambda}(\mathbf{k}) a_{\mathbf{k}}^{\dagger}(\tau) a_{\mathbf{k}}(\tau)} e^{\int_0^\beta d\tau \sum_{\mathbf{k}} \left[\bar{\jmath}_{\mathbf{k}}(\tau) a_{\mathbf{k}}(\tau) + a_{\mathbf{k}}^{\dagger}(\tau) j_{\mathbf{k}}(\tau) \right] \right] \right\}}.$$
(2.14)

Taking the derivative $\partial_{\Lambda}\Gamma_{\Lambda}[\bar{\psi},\psi]$ and substituting for $\partial_{\Lambda}\mathcal{G}_{\Lambda}[\bar{j},j]$ the flow equation (2.11), we find

$$\partial_{\Lambda}\Gamma_{\Lambda}[\bar{\psi},\psi] = \zeta \int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\partial_{\Lambda}R_{\Lambda}(\mathbf{k})\right] \frac{\delta^{2}\mathcal{G}_{\Lambda}[j,j]}{\delta j_{\mathbf{k}}(\tau)\delta\bar{j}_{\mathbf{k}}(\tau)}.$$

To derive the usual form of the Wetterich equation 6, we adopt the super-field notation developed in Refs. 3 and 19: for our model describing spinless fermions or bosons

this amounts to introducing a two-component field

$$(\Phi_{\alpha}) = \begin{pmatrix} \Phi_{(\psi k\tau)} \\ \Phi_{(\bar{\psi}k\tau)} \end{pmatrix} = \begin{pmatrix} \psi_{k}(\tau) \\ \bar{\psi}_{k}(\tau) \end{pmatrix}, \qquad (2.16)$$

where the super-label $\alpha=(pk\tau)$ denotes all parameters which are necessary to completely specify the field combination. Here, $p=\psi,\bar{\psi}$ keeps track of the field type. As shown in Ref. 8, the second functional derivative in

Eq. (2.15) can then be expressed in terms of the second derivative matrix of $\Gamma_{\Lambda}[\bar{\psi}, \psi]$ as follows:

$$\frac{\delta^{2} \mathcal{G}_{\Lambda}[\bar{j},j]}{\delta j_{\mathbf{k}}(\tau) \delta \bar{j}_{\mathbf{k}}(\tau)}
= \left[\left(\frac{\delta}{\delta \Phi} \otimes \frac{\delta}{\delta \Phi} \right)^{T} \Gamma_{\Lambda}[\bar{\psi},\psi] + \mathbf{R}_{\Lambda} \right]_{\alpha = (\psi \mathbf{k} \tau), \alpha' = (\bar{\psi} \mathbf{k} \tau)}^{-1},$$
(2.17)

where the matrix elements of the second derivative operators $\frac{\delta}{\delta\Phi}\otimes\frac{\delta}{\delta\Phi}$ in super-field space is defined by

$$\left[\frac{\delta}{\delta\Phi} \otimes \frac{\delta}{\delta\Phi}\right]_{\alpha\alpha'} = \frac{\delta}{\delta\Phi_{\alpha}} \frac{\delta}{\delta\Phi_{\alpha'}},\tag{2.18a}$$

$$\left[\frac{\delta}{\delta\Phi} \otimes \frac{\delta}{\delta\Phi}\right]_{\alpha\alpha'}^{T} = \frac{\delta}{\delta\Phi_{\alpha'}} \frac{\delta}{\delta\Phi_{\alpha}} = \zeta \frac{\delta}{\delta\Phi_{\alpha}} \frac{\delta}{\delta\Phi_{\alpha'}}.$$
 (2.18b)

Note that for fermions where the Φ_{α} anticommute the transposition in Eq. (2.18b) generates an extra factor of $\zeta = -1$. The regulator matrix \mathbf{R}_{Λ} in superfield space in Eq. (2.17) is defined by writing the regulator term in Eq. (2.12) in (anti)-symmetrized superfield notation [8],

$$\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} R_{\Lambda}(\mathbf{k}) \bar{\psi}_{\mathbf{k}}(\tau) \psi_{\mathbf{k}}(\tau) = \frac{1}{2} \int_{\alpha} \int_{\beta} \Phi_{\alpha}[\mathbf{R}_{\Lambda}]_{\alpha\alpha'} \Phi_{\alpha'},$$
(2.19)

where $\int_{\alpha} = \sum_{p=\psi,\bar{\psi}} \sum_{\mathbf{k}} \int_{0}^{\beta} d\tau$ denotes summation or integration over all components of the superfield label. Substituting Eq. (2.17) into the flow equation (2.15), we finally obtain the Wetterich equation for the average effective action, $\Gamma_{\Lambda}[\Phi] = \Gamma_{\Lambda}[\bar{\psi}, \psi]$ in the form

$$\begin{split} \partial_{\Lambda}\Gamma_{\Lambda}[\Phi] &= \\ \frac{\zeta}{2}\mathrm{Tr}\left\{ (\partial_{\Lambda}\mathbf{R}_{\Lambda}) \left[\left(\frac{\delta}{\delta\Phi} \otimes \frac{\delta}{\delta\Phi} \right)^{T} \Gamma_{\Lambda}[\Phi] + \mathbf{R}_{\Lambda} \right]^{-1} \right\}, \end{split}$$

$$(2.20)$$

where the trace is over all labels contained in the superfield label α . Note that nowhere in our derivation of the Wetterich equation (2.20) we have used functional integrals. Our derivation of the Wetterich equation for quantum spin systems presented in Ref. [7] relies on the same sequence of manipulations. Evidently, this strategy can also be used to derive (generalized) Wetterich equations for other quantum systems whose Hamiltonian is defined in terms of operators satisfying non-canonical commutation relations.

Since in Eq. (2.7) we have introduced the regulator $R_{\Lambda}(\mathbf{k})$ directly in the Hamiltonian, it seems at first sight that the flexibility of introducing a frequency-dependent regulator in a functional integral approach is lost within our operator formalism. This is not true, however, because we can alternatively introduce the regulator directly in the generating functional $\mathcal{G}_{\Lambda}[\bar{j},j]$ of connected correlation functions, so that the original generating

functional in Eq. (2.9) is replaced by the deformed functional

$$e^{\mathcal{G}_{\Lambda}[\bar{j},j]} = \operatorname{Tr} \left\{ e^{-\beta \tilde{\mathcal{H}}} \mathcal{T} \left[e^{-\int_{0}^{\beta} d\tau d\tau' \sum_{\mathbf{k}} R_{\Lambda}(\mathbf{k},\tau-\tau') a_{\mathbf{k}}^{\dagger}(\tau) a_{\mathbf{k}}(\tau')} \right. \right. \\ \left. \times e^{\int_{0}^{\beta} d\tau \sum_{\mathbf{k}} \left[\bar{j}_{\mathbf{k}}(\tau) a_{\mathbf{k}}(\tau) + a_{\mathbf{k}}^{\dagger}(\tau) j_{\mathbf{k}}(\tau) \right]} \right] \right\},$$

$$(2.21)$$

where $R_{\Lambda}(\mathbf{k}, \tau - \tau')$ is the imaginary-time Fourier transform of a general frequency-dependent regulator $R_{\Lambda}(\mathbf{k}, i\omega)$; i.e.,

$$R_{\Lambda}(\mathbf{k}, \tau - \tau') = \frac{1}{\beta} \sum_{\omega} e^{-i\omega(\tau - \tau')} R_{\Lambda}(\mathbf{k}, i\omega).$$
 (2.22)

III. HUBBARD X-OPERATORS

A. Hubbard model

The Hubbard model is defined by the following second quantized lattice Hamiltonian [20, [21]:

$$\mathcal{H} = \sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \qquad (3.1)$$

where $c_{i\sigma}$ is the canonical annihilation operator of an electron with spin projection $\sigma=\uparrow,\downarrow$ at lattice site r_i . The corresponding creation operator is denoted by $c_{i\sigma}^{\dagger}$ and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$ is the occupation number operator. For each lattice site, the Hilbert space is spanned by four states $|i,0\rangle, |i,\uparrow\rangle = c_{i\uparrow}^{\dagger}|i,0\rangle, |i,\downarrow\rangle = c_{i\downarrow}^{\dagger}|i,0\rangle$, and $|i,2\rangle = c_{i\downarrow}^{\dagger}c_{i\uparrow}^{\dagger}|i,0\rangle = -c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger}|i,0\rangle$ that describe lattice sites which are either empty, occupied by a single electron with spin $\sigma=\uparrow,\downarrow$, or occupied by two electrons with opposite spin. We denote the states by $|i,a\rangle$ with $a\in\{0,\uparrow,\downarrow,2\}$. The X-operators X_i^{ab} act on the single-site Fock space and can be defined as follows 15-17:

$$X_i^{ab} = |i, a\rangle \langle i, b|. \tag{3.2}$$

This set of 16 operators describes all possible transitions between the four states of the single-site Fock space. The X-operators can be further subdivided into a subset of eight Fermi type operators and eight Bose type operators. The Fermi type X-operators can be expressed in terms of an odd number of fermionic annihilation or creation operators,

$$X_i^{\sigma 0} = c_{i\sigma}^{\dagger} (1 - n_{i\bar{\sigma}}), \tag{3.3a}$$

$$X_i^{0\sigma} = (X_i^{\sigma 0})^{\dagger} = (1 - n_{i\bar{\sigma}})c_{i\sigma},$$
 (3.3b)

$$X_i^{2\sigma} = \sigma c_{i\bar{\sigma}}^{\dagger} n_{i\sigma}, \tag{3.3c}$$

$$X_i^{\sigma 2} = (X_i^{2\sigma})^{\dagger} = \sigma n_{i\sigma} c_{i\bar{\sigma}}, \tag{3.3d}$$

where $\sigma = \uparrow, \downarrow = +, -$ labels the two spin projections and $\bar{\sigma} = -\sigma$ represents the spin projection opposite to σ .

Note that for Fermi type X-operators X_i^{ab} the number of electrons in the two states $|i,a\rangle$ and $|i,b\rangle$ differs by an odd number. Equation (3.3) implies that the canonical Fermi operators $c_{i\sigma}$ and $c_{i\sigma}^{\dagger}$ can be expressed in terms of the Fermi type X-operators as follows:

$$c_{i\sigma} = X_i^{0\sigma} - \sigma X_i^{\bar{\sigma}2}, \qquad c_{i\sigma}^{\dagger} = X_i^{\sigma 0} - \sigma X_i^{2\bar{\sigma}}.$$
 (3.4)

The remaining eight X-operators X_i^{ab} are of the Bose type. This means that the states $|i,a\rangle$ and $|i,b\rangle$ differ by an even number of electrons; these operators can consequently be expressed in terms of an even number of annihilation or creation operators,

$$X_i^{\sigma\bar{\sigma}} = c_{i\sigma}^{\dagger} c_{i\bar{\sigma}}, \quad \sigma = \uparrow, \downarrow,$$
 (3.5a)

$$X_i^{\sigma\sigma} = n_{i\sigma}(1 - n_{i\bar{\sigma}}), \quad \sigma = \uparrow, \downarrow,$$
 (3.5b)

$$X_i^{00} = (1 - n_{i\uparrow})(1 - n_{i\downarrow}),$$
 (3.5c)

$$X_i^{22} = n_{i\uparrow} n_{i\downarrow}, \tag{3.5d}$$

$$X_i^{20} = c_i^{\dagger} c_{i\uparrow}^{\dagger}, \tag{3.5e}$$

$$X_i^{02} = (X_i^{20})^{\dagger} = c_{i\uparrow}c_{i\downarrow}.$$
 (3.5f)

From the definition (3.2) we see that the product of two X-operators associated with the same lattice site can be expressed in terms of another X-operator,

$$X_i^{ab} X_i^{cd} = \delta_{bc} X_i^{ad}. \tag{3.6}$$

This product rule together with the anticommutation relations of the fermionic creation and annihilation operators at different sites defines the algebra of the Xoperators. Any pair of Fermi type X-operators satisfies the anti-commutation relations

$$[X_i^{ab}, X_j^{cd}]_+ = \delta_{ij} \left(\delta_{bc} X_i^{ad} + \delta_{da} X_i^{cb} \right).$$
 (3.7)

On the other hand, a pair of Bose type X-operators or a pair consisting of one Bose type X-operator and one Fermi type X-operator satisfies the commutation relations

$$[X_i^{ab}, X_j^{cd}] = \delta_{ij} \left(\delta_{bc} X_i^{ad} - \delta_{da} X_i^{cb} \right). \tag{3.8}$$

Finally, the completeness of the four-dimensional singlesite Fock space implies the sum rule

$$\sum_{a} X_i^{aa} = \sum_{a} |i, a\rangle \langle i, a| = 1.$$
 (3.9)

In principle one could require that for different sites all X-operators commute [22], but then the representation (3.3) of the Fermi type X-operators in terms of canonical fermions would not be valid. The underlying reason for choosing the anticommutation relations (3.7) for the Fermi type X-operators is the physical requirement that the many-body electronic wave function has to be totally antisymmetric with respect to exchange of any two electrons. The anticommutation relations (3.7) together with the commutation relations (3.8) define the semi-simple

doubly graded (supersymmetrical) Lie algebra Spl(1,2) [23]. The representations (3.3) and (3.5) associate the type assignments of the X-operators with the number of canonical fermions: Fermi type X-operators can be expressed in terms of an odd number of canonical Fermi operators, while Bose type X-operators can be expressed in terms of an even number of canonical Fermi operators. Note that this assignment does not agree with the classification scheme given by Tsvelik [24].

Using Eqs. (3.5d) and (3.4), we can express the Hubbard Hamiltonian (3.1) in terms of the X-operators as follows:

$$\mathcal{H} = U \sum_{i} X_i^{22} + \mathcal{H}_2,$$
 (3.10)

where the first part represents the on-site interaction and the kinetic energy represented by the second part \mathcal{H}_2 can be written as

$$\mathcal{H}_{2} = \sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma}$$

$$= \sum_{ij\sigma} t_{ij} \left(X_{i}^{\sigma 0} - \sigma X_{i}^{2\bar{\sigma}} \right) \left(X_{j}^{0\sigma} - \sigma X_{j}^{\bar{\sigma}2} \right)$$

$$= \sum_{ij\sigma} t_{ij} \left(X_{i}^{\sigma 0} X_{j}^{0\sigma} + X_{i}^{2\bar{\sigma}} X_{j}^{\bar{\sigma}2} + \bar{\sigma} X_{i}^{\sigma 0} X_{j}^{\bar{\sigma}2} + \bar{\sigma} X_{i}^{2\bar{\sigma}} X_{j}^{0\sigma} \right)$$

$$= \sum_{ij\sigma} t_{ij} \psi_{i\sigma}^{\dagger} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \psi_{j\sigma} = \sum_{ij\sigma} \psi_{i\sigma}^{\dagger} \hat{t}_{ij} \psi_{j\sigma}. \tag{3.11}$$

Here, we have introduced the two-flavor Fermi-like operators

$$\psi_{i\sigma} = \begin{pmatrix} X_i^{0\sigma} \\ \bar{\sigma} X_i^{\bar{\sigma}2} \end{pmatrix}, \qquad \psi_{i\sigma}^{\dagger} = \begin{pmatrix} X_i^{\sigma 0}, \bar{\sigma} X_i^{2\bar{\sigma}} \end{pmatrix}, \qquad (3.12)$$

and the 2×2 hopping matrix in flavor space,

$$\hat{t}_{ij} = t_{ij} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \tag{3.13}$$

Alternatively, introducing the four-component operators

$$\phi_{i\sigma} = \begin{pmatrix} X_i^{0\sigma} \\ \bar{\sigma} X_i^{\bar{\sigma}2} \\ X_i^{\sigma 0} \\ \bar{\sigma} X_i^{2\bar{\sigma}} \end{pmatrix}, \tag{3.14}$$

the kinetic energy operator can be written in the manifestly antisymmetric form

$$\mathcal{H}_{2} = \frac{1}{2} \sum_{ij\sigma} \phi_{i\sigma}^{T} \begin{pmatrix} 0 & 0 & -1 & -1 \\ 0 & 0 & -1 & -1 \\ \hline 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix} \phi_{j\sigma}.$$
 (3.15)

Finally, the particle number operator can be written as

$$\mathcal{N} = \sum_{i\sigma} n_{i\sigma} = \sum_{i} \left(X_i^{\uparrow\uparrow} + X_i^{\downarrow\downarrow} + 2X_i^{22} \right), \qquad (3.16)$$

so that the grand canonical Hamiltonian of the Hubbard model is of the form $\tilde{\mathcal{H}} = \mathcal{H}_1 + \mathcal{H}_2$ as given in Eq. (2.4), with \mathcal{H}_2 given in Eq. (3.11) and

$$\mathcal{H}_1 = \sum_{ia} \epsilon_a X_i^{aa}, \tag{3.17}$$

with $\epsilon_0 = 0$, $\epsilon_{\uparrow} = \epsilon_{\downarrow} = -\mu$, and $\epsilon_2 = U - 2\mu$. In the presence of an external magnetic field the Zeemann energy h lifts the degeneracy between ϵ_{\uparrow} and ϵ_{\downarrow} so that $\epsilon_{\sigma} = -\mu - \sigma h/2$.

B. t-J model

The t-J model is an effective model for electrons hopping on a lattice with strong on-site interactions such that states with doubly occupied sites are not accessible. The Hamiltonian of the t-J model acts on a projected Hilbert space defined by the Fock space spanned by the three states $|i,0\rangle, |i,\uparrow\rangle = c^{\dagger}_{i\uparrow}|i,0\rangle$, and $|i,\downarrow\rangle = c^{\dagger}_{i\downarrow}|i,0\rangle$. The Hamiltonian of the t-J model is [20] [21]

$$\mathcal{H}_{tJ} = \sum_{ij\sigma} t_{ij} \tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{j\sigma} + \frac{1}{2} \sum_{ij} J_{ij} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{\tilde{n}_i \tilde{n}_j}{4} \right),$$
(3.18)

where

$$\tilde{c}_{i\sigma}^{\dagger} = c_{i\sigma}^{\dagger} (1 - n_{i\bar{\sigma}}) = X_i^{\sigma 0}, \tag{3.19a}$$

$$\tilde{c}_{i\sigma} = (1 - n_{i\bar{\sigma}})c_{i\sigma} = X_i^{0\sigma} \tag{3.19b}$$

are projected Fermi operators acting on the restricted Hilbert space of states without doubly occupied lattice sites, and the spin operators and the projected particle number operators are defined by

$$\mathbf{S}_{i} = \frac{1}{2} \left(\tilde{c}_{i\uparrow}^{\dagger}, \tilde{c}_{i\downarrow}^{\dagger} \right) \boldsymbol{\sigma} \left(\begin{array}{c} \tilde{c}_{i\uparrow} \\ \tilde{c}_{i\downarrow} \end{array} \right), \tag{3.20}$$

$$\tilde{n}_i = \sum_{\sigma} \tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{i\sigma} = \sum_{\sigma} n_{i\sigma} (1 - n_{i\bar{\sigma}}) = \sum_{\sigma} X_i^{\sigma\sigma}. \quad (3.21)$$

Here, the components of the vector σ are the usual Pauli matrices. Using the identities

$$S_i^+ = S_i^x + iS_i^y = \tilde{c}_{i\uparrow}^{\dagger} \tilde{c}_{i\downarrow} = c_{i\uparrow}^{\dagger} c_{i\downarrow} = X_i^{+-}, \qquad (3.22a)$$

$$S_i^- = S_i^x - iS_i^y = \tilde{c}_{i\downarrow}^{\dagger} \tilde{c}_{i\uparrow} = c_{i\downarrow}^{\dagger} c_{i\uparrow} = X_i^{-+}, \qquad (3.22b)$$

$$S_i^z = \frac{1}{2} \left[\tilde{n}_{i\uparrow} - \tilde{n}_{i\downarrow} \right] = \frac{1}{2} \left[n_{i\uparrow} (1 - n_{i\downarrow}) - n_{i\downarrow} (1 - n_{i\uparrow}) \right]$$
$$= \frac{1}{2} \left[n_{i\uparrow} - n_{i\downarrow} \right] = \frac{1}{2} \sum_{\sigma} \sigma X_i^{\sigma\sigma}, \tag{3.22c}$$

and

$$S_i^z S_j^z - \frac{\tilde{n}_i \tilde{n}_j}{4} = -\frac{1}{2} \left[n_{i\uparrow} (1 - n_{i\downarrow}) n_{j\downarrow} (1 - n_{i\uparrow}) + n_{i\downarrow} (1 - n_{i\uparrow}) n_{j\uparrow} (1 - n_{i\downarrow}) \right]$$
$$= -\frac{1}{2} \sum_{\sigma} X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}}, \qquad (3.23)$$

we see that in terms of X-operators the t-J Hamiltonian assumes the form

$$\mathcal{H}_{tJ} = \sum_{ij\sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma} + \frac{1}{4} \sum_{ij\sigma} J_{ij} \left(X_i^{\sigma \bar{\sigma}} X_j^{\bar{\sigma}\sigma} - X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}} \right). \tag{3.24}$$

Using the completeness relation in the projected Hilbert space,

$$X_i^{00} + X_i^{\uparrow\uparrow} + X_i^{\downarrow\downarrow} = 1, \tag{3.25}$$

we may write

$$\begin{split} X_i^{00} X_j^{00} &= 1 - \sum_{\sigma} \left(X_i^{\sigma\sigma} + X_j^{\sigma\sigma} \right) \\ &+ \sum_{\sigma} \left(X_i^{\sigma\sigma} X_j^{\sigma\sigma} + X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}} \right), \end{split} \tag{3.26}$$

and hence

$$\begin{split} \sum_{\sigma} X_{i}^{\sigma\sigma} X_{j}^{\bar{\sigma}\bar{\sigma}} &= X_{i}^{00} X_{j}^{00} - \sum_{\sigma} X_{i}^{\sigma\sigma} X_{j}^{\sigma\sigma} \\ &+ \sum_{\sigma} \left(X_{i}^{\sigma\sigma} + X_{j}^{\sigma\sigma} \right) - 1. \end{split} \tag{3.27}$$

Using the anticommutation relation $X_j^{\sigma 0}X_i^{0\sigma} = -X_i^{0\sigma}X_j^{\sigma 0}$ for $i \neq j$ we can alternatively write the t-J Hamiltonian in terms of X-operators as follows:

$$\mathcal{H}_{tJ} = \frac{1}{2} \sum_{ij\sigma} t_{ij} \left(X_i^{0\sigma} X_j^{\sigma 0} - X_i^{\sigma 0} X_j^{0\sigma} \right)$$

$$+ \frac{1}{4} \sum_{ij} J_{ij} \left[-X_i^{00} X_j^{00} + \sum_{\sigma\sigma'} X_i^{\sigma\sigma'} X_j^{\sigma'\sigma} \right]$$

$$+ \frac{1}{4} \sum_{ij} J_{ij} \left(X_i^{00} - \sum_{\sigma} X_i^{\sigma\sigma} \right), \qquad (3.28)$$

where in the last term we have used the operator identity (3.25) to write

$$\sum_{ij} J_{ij} \left[1 - \sum_{\sigma} \left(X_i^{\sigma\sigma} + X_j^{\sigma\sigma} \right) \right]$$

$$= \sum_{ij} J_{ij} \left(X_i^{00} - \sum_{\sigma} X_j^{\sigma\sigma} \right)$$

$$= \sum_{ij} J_{ij} \left(X_i^{00} - \sum_{\sigma} X_i^{\sigma\sigma} \right). \tag{3.29}$$

For completeness let us mention that for nearest neighbor hopping and exchange where $t_{ij} = -t$ and $J_{ij} = J$ for all pairs of nearest neighbors on a square lattice, there is a special supersymmetric point t = J/2 where the t-J Hamiltonian (3.28) exhibits an enhanced symmetry and can be written as [23] [25] [26]

$$\mathcal{H}_{tJ}^{\text{SUSY}} = \frac{J}{2} \sum_{\langle ij \rangle} \left[\sum_{ab} \zeta_b X_i^{ab} X_j^{ba} - \sum_a \zeta_a X_i^{aa} \right], \quad (3.30)$$

where $a, b \in \{0, +, -\}$ and we have introduced the statistics factors $\zeta_0 = -1$ and $\zeta_+ = \zeta_- = 1$.

\mathbf{C} . t model

In the extreme strong-coupling limit $J \to 0$, the t-J Hamiltonian reduces to the t model consisting only of the projected kinetic energy,

$$\mathcal{H}_t = \sum_{ij\sigma} t_{ij} \tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{j\sigma} = \sum_{ij\sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma}, \tag{3.31}$$

which can be obtained from the Hubbard model in the limit of infinite on-site repulsion U. Due to the projected Hilbert space the correlation functions of the t model are non-trivial; see Ref. 27 for a calculation of the densitydensity and spin-spin correlation functions of the t model within a 1/N expansion. Moreover, the single-particle Green function of the projected fermions is also expected to be dominated by the strong kinematic constraints due to the Hilbert space projection. In fact, according to the late P. W. Anderson 28+30, in two dimensions the projected kinetic energy represented by the t model is an effective Hamiltonian describing the normal metallic state of the cuprate superconductors, which he called a "hidden Fermi liquid". In Sec. VB we will use our X-FRG approach to calculate the quasi-particle damping in the hidden Fermi liquid.

IV. EXACT X-FRG FLOW EQUATIONS

The grand canonical Hamiltonian of each of the models introduced in Sec. \boxed{III} can be written in the form $\tilde{\mathcal{H}} = \mathcal{H}_1 + \mathcal{H}_2$, where the single-site term \mathcal{H}_1 is linear in the X-operators and the hopping term \mathcal{H}_2 is quadratic and involves pairs of X-operators at different lattice sites. Following the same strategy as in the derivation of FRG flow equations for quantum spin systems $\boxed{7}$, we now replace the inter-site hopping t_{ij} in \mathcal{H}_2 by a deformed hopping $t_{ij,\Lambda}$ depending on a continuous parameter Λ , which we parametrize as

$$t_{ij,\Lambda} = t_{ij} + R_{ij,\Lambda}^t. \tag{4.1}$$

The regulator function $R_{ij,\Lambda}^t$ should be chosen such that for some initial value $\Lambda=0$ the deformed model simplifies so that its correlation functions can be calculated in a controlled way, while $t_{ij,\Lambda} \to t_{ij}$ for $\Lambda \to 1$, so that in this limit we recover our original model. For the t-J model, we similarly replace the exchange coupling by a deformed coupling

$$J_{ij,\Lambda} = J_{ij} + R_{ij,\Lambda}^J. \tag{4.2}$$

The deformed grand canonical Hamiltonian is then

$$\tilde{\mathcal{H}}_{\Lambda} = \mathcal{H}_1 + \mathcal{H}_{2,\Lambda},$$
 where \mathcal{H}_1 is of the form (3.17). For the Hubbard model,

where \mathcal{H}_1 is of the form (3.17). For the Hubbard model, the deformed hopping term is given by the deformed kinetic energy,

$$\mathcal{H}_{2,\Lambda} = \sum_{ij\sigma} t_{ij,\Lambda} \left(X_i^{\sigma 0} X_j^{0\sigma} + X_i^{2\bar{\sigma}} X_j^{\bar{\sigma}2} + \bar{\sigma} X_i^{\sigma 0} X_j^{\bar{\sigma}2} + \bar{\sigma} X_i^{2\bar{\sigma}} X_j^{0\sigma} \right). \tag{4.4}$$

In the case of the t-J model, we should omit all X-operators involving doubly occupied sites and add the exchange interaction involving Bose type X-operators; using the representation (3.24) we find for the hopping contribution to the deformed t-J Hamiltonian

$$\mathcal{H}_{2,\Lambda} = \sum_{ij\sigma} t_{ij,\Lambda} X_i^{\sigma 0} X_j^{0\sigma} + \frac{1}{4} \sum_{ij\sigma} J_{ij,\Lambda} \left(X_i^{\sigma \bar{\sigma}} X_j^{\bar{\sigma}\sigma} - X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}} \right). \tag{4.5}$$

For both models, the deformed generating functional of connected imaginary-time ordered X-operator correlation functions can be written as a trace of a time-ordered exponential,

$$e^{\mathcal{G}_{\Lambda}[J]} = \operatorname{Tr}\left[e^{-\beta\mathcal{H}_{1}}\mathcal{T}e^{-\int_{0}^{\beta}d\tau\mathcal{H}_{2,\Lambda}(\tau)}e^{\int_{0}^{\beta}d\tau\sum_{i,p}J_{i}^{p}(\tau)X_{i}^{p}(\tau)}\right],$$

$$(4.6)$$

where $\mathcal{H}_{2,\Lambda}$ is obtained from the inter-site part \mathcal{H}_2 of the Hamiltonian by replacing the hopping and the exchange coupling by the deformed quantities, and the time-dependence of all operators is in the interaction picture with respect to \mathcal{H}_1 . The label p enumerates all types of X-operators; i.e., $p=1,\ldots,16$ for the Hubbard model and $p=1,\ldots,9$ for the t-J model. Because Bose (Fermi) type X-Operators (anti-)commute at different lattice sites, the sources $J_i^p(\tau)$ are Grassmann variables for Fermi type X-operators and complex variables for Bose type X-operators. For the same reason, the time-ordering of Bose (Fermi) type X-operators is defined as for canonical bosons (fermions).

A. Flow equation for the Hubbard model

To derive an exact flow equation for $\mathcal{G}_{\Lambda}[J]$ we proceed as in Eq. (2.10) and take a derivative of both sides of Eq. (4.6) with respect to the deformation parameter Λ . For the Hubbard model, we obtain

$$e^{\mathcal{G}_{\Lambda}[J]}\partial_{\Lambda}\mathcal{G}_{\Lambda}[J] = -\int_{0}^{\beta}d\tau \sum_{ij\sigma} \left(\partial_{\Lambda}t_{ij,\Lambda}\right) \operatorname{Tr} \left\{ e^{-\beta\mathcal{H}_{1}}\mathcal{T} \left[e^{-\int_{0}^{\beta}d\tau\mathcal{H}_{2,\Lambda}(\tau)} \left(X_{i}^{\sigma0}(\tau) X_{j}^{0\sigma}(\tau) + X_{i}^{2\bar{\sigma}}(\tau) X_{j}^{\bar{\sigma}^{2}}(\tau) \right) \right. \\ \left. + \bar{\sigma} X_{i}^{\sigma0}(\tau) X_{j}^{\bar{\sigma}^{2}}(\tau) + \bar{\sigma} X_{i}^{2\bar{\sigma}}(\tau) X_{j}^{0\sigma}(\tau) \right) e^{\int_{0}^{\beta}d\tau \sum_{i,p} J_{i}^{p}(\tau) X_{i}^{p}(\tau)} \right] \right\}$$

$$\left. + \bar{\sigma} X_{i}^{\sigma0}(\tau) X_{j}^{\bar{\sigma}^{2}}(\tau) + \bar{\sigma} X_{i}^{2\bar{\sigma}}(\tau) X_{j}^{0\sigma}(\tau) + \frac{\delta}{\delta J_{i}^{2\bar{\sigma}}(\tau)} \frac{\delta}{\delta J_{j}^{\bar{\sigma}^{2}}(\tau)} \right. \\ \left. + \frac{\delta}{\delta J_{i}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\bar{\sigma}^{2}}(\tau)} + \bar{\sigma} \frac{\delta}{\delta J_{i}^{2\bar{\sigma}}(\tau)} \frac{\delta}{\delta J_{j}^{0\sigma}(\tau)} \right) e^{\int_{0}^{\beta}d\tau \sum_{i,p} J_{i}^{p}(\tau) X_{i}^{p}(\tau)} \right] \right\}$$

$$\left. + \bar{\sigma} \frac{\delta}{\delta J_{i}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\bar{\sigma}^{2}}(\tau)} + \bar{\sigma} \frac{\delta}{\delta J_{i}^{2\bar{\sigma}}(\tau)} \frac{\delta}{\delta J_{j}^{\bar{\sigma}^{2}}(\tau)} \right) e^{\int_{0}^{\beta}d\tau \sum_{i,p} J_{i}^{p}(\tau) X_{i}^{p}(\tau)} \right] \right\}$$

$$\left. + \bar{\sigma} \frac{\delta}{\delta J_{i}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\bar{\sigma}^{2}}(\tau)} + \bar{\sigma} \frac{\delta}{\delta J_{i}^{\bar{\sigma}^{2}}(\tau)} \frac{\delta}{\delta J_{j}^{\bar{\sigma}^{2}}(\tau)} \frac{\delta}{\delta J_{j}^{\bar{\sigma}^{2}}(\tau)} \right) e^{\int_{0}^{\beta}d\tau \sum_{i,p} J_{i}^{p}(\tau) X_{i}^{p}(\tau)} \right] \right\}$$

$$\left. + \bar{\sigma} \frac{\delta}{\delta J_{i}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\sigma0}(\tau)} + \bar{\sigma} \frac{\delta}{\delta J_{i}^{\bar{\sigma}^{2}}(\tau)} \frac{\delta}{\delta J_{j}^{\bar{\sigma}^{2}}(\tau)} \right) e^{\int_{0}^{\beta}d\tau \sum_{i,p} J_{i}^{p}(\tau) X_{i}^{p}(\tau)} \right] \right\}$$

$$\left. + \bar{\sigma} \frac{\delta}{\delta J_{i}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\sigma0}(\tau)} \right) e^{\int_{0}^{\beta}d\tau \sum_{i,p} J_{i}^{p}(\tau) X_{i}^{p}(\tau)} \right] \right\}$$

$$\left. + \bar{\sigma} \frac{\delta}{\delta J_{i}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{i}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\sigma0}(\tau)} \frac{\delta}{\delta J_{j}^{\sigma0}(\tau)} \right) e^{\int_{0}^{\beta}d\tau \sum_{i,p} J_{i}^{p}(\tau) X_{i}^{p}(\tau)} \left(\frac{\delta}{\delta J_{i}^{\sigma0}(\tau)} \right) e^{\int_{0}^{\beta}d\tau \sum_{i,p} J_{i}^{\rho0}(\tau) \frac{\delta}{\delta J_{i}^{\sigma0}(\tau)} \frac{\delta}{\delta$$

We conclude that the generating functional of the connected imaginary-time ordered X-operator correlation functions of the Hubbard model satisfies the exact flow equation

$$\partial_{\Lambda}\mathcal{G}_{\Lambda}[J] = -\int_{0}^{\beta} d\tau \sum_{ij\sigma} \left(\partial_{\Lambda}t_{ij,\Lambda}\right) \left\{ \frac{\delta^{2}\mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\sigma0}(\tau)\delta J_{j}^{0\sigma}(\tau)} + \frac{\delta\mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\sigma0}(\tau)} \frac{\delta\mathcal{G}_{\Lambda}[J]}{\delta J_{j}^{0\sigma}(\tau)} + \frac{\delta^{2}\mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{2\bar{\sigma}}(\tau)\delta J_{j}^{\bar{\sigma}2}(\tau)} + \frac{\delta\mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{2\bar{\sigma}}(\tau)\delta J_{j}^{\bar{\sigma}2}(\tau)} + \frac{\delta\mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\bar{\sigma}2}(\tau)} \frac{\delta\mathcal{G}_{\Lambda}[J]}{\delta J_{j}^{\bar{\sigma}2}(\tau)} + \bar{\sigma} \frac{\delta^{2}\mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\bar{\sigma}2}(\tau)\delta J_{j}^{\bar{\sigma}2}(\tau)} + \bar{\sigma} \frac{\delta\mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\bar{\sigma}2}(\tau)\delta J_{j}^{\bar{\sigma}2}(\tau)} \right\}.$$
(4.8)

Next, we introduce the subtracted Legendre transform of $\mathcal{G}_{\Lambda}[J]$ via

$$\Gamma_{\Lambda}[\bar{X}] = \int_{0}^{\beta} d\tau \sum_{i,p} J_{i}^{p}(\tau) \bar{X}_{i}^{p}(\tau) - \mathcal{G}_{\Lambda}[J]$$

$$- \int_{0}^{\beta} d\tau \sum_{ij\sigma} R_{ij,\Lambda}^{t} \left[\bar{X}_{i}^{\sigma 0}(\tau) \bar{X}_{j}^{0\sigma}(\tau) + \bar{X}_{i}^{2\bar{\sigma}}(\tau) \bar{X}_{j}^{\bar{\sigma}2}(\tau) \right]$$

$$+ \bar{\sigma} \bar{X}_{i}^{\sigma 0}(\tau) \bar{X}_{j}^{\bar{\sigma}2}(\tau) + \bar{\sigma} \bar{X}_{i}^{2\bar{\sigma}}(\tau) \bar{X}_{j}^{0\sigma}(\tau) \right], \quad (4.9)$$

where on the right-hand side the sources $J_i^p(\tau)$ should be expressed in terms of the expectation values $\bar{X}_i^p(\tau)$ by inverting the relation

$$\bar{X}_{i}^{p}(\tau) = \langle \mathcal{T}X_{i}^{p}(\tau) \rangle = \frac{\delta \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{p}(\tau)}.$$
 (4.10)

Using the flow equation (4.8) we find that the functional $\Gamma_{\Lambda}[\bar{X}]$ satisfies the exact flow equation

$$\partial_{\Lambda}\Gamma_{\Lambda}[\bar{X}] = \int_{0}^{\beta} d\tau \sum_{ij\sigma} \left(\partial_{\Lambda} R_{ij,\Lambda}^{t}\right)$$

$$\times \left[\frac{\delta^{2} \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\sigma 0}(\tau) \delta J_{j}^{0\sigma}(\tau)} + \frac{\delta^{2} \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{2\bar{\sigma}}(\tau) \delta J_{\bar{j}}^{\bar{\sigma}^{2}}(\tau)} + \bar{\sigma} \frac{\delta^{2} \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\sigma 0}(\tau) \delta J_{\bar{j}}^{\bar{\sigma}^{2}}(\tau)} + \bar{\sigma} \frac{\delta^{2} \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{2\bar{\sigma}}(\tau) \delta J_{j}^{0\sigma}(\tau)}\right]. \quad (4.11)$$

To compactify the notation, we now collect all X-operators into a 16-component vector

$$(\Phi_{\alpha}) = \begin{pmatrix} \Phi_{\uparrow} \\ \Phi_{\downarrow} \\ \Phi_{0} \\ \Phi_{2} \end{pmatrix}, \tag{4.12}$$

where the four-component vectors Φ_{\uparrow} and Φ_{\downarrow} contain the expectation values of the Fermi type X-operators,

$$\Phi_{\sigma} = \begin{pmatrix} \bar{X}^{0\sigma} \\ \bar{\sigma}\bar{X}^{\bar{\sigma}2} \\ \bar{X}^{\sigma 0} \\ \bar{\sigma}\bar{X}^{2\bar{\sigma}} \end{pmatrix}, \qquad \sigma = \uparrow, \downarrow, \tag{4.13}$$

while the four-component vectors Φ_0 and Φ_2 contain the expectation values of the Bose type X-operators as follows:

$$\Phi_0 = \begin{pmatrix} \bar{X}^{\uparrow\uparrow} \\ \bar{X}^{\downarrow\downarrow} \\ \bar{X}^{\uparrow\downarrow} \\ \bar{X}^{\downarrow\uparrow} \end{pmatrix}, \qquad \Phi_2 = \begin{pmatrix} \bar{X}^{00} \\ \bar{X}^{02} \\ \bar{X}^{20} \\ \bar{X}^{22} \end{pmatrix}.$$
(4.14)

For simplicity we have omitted the lattice site and imaginary time labels. The derivation of the Wetterich equation follows precisely the same steps as the derivation for

canonical bosons or fermions outlined in Sec. \blacksquare The only difference is that now the superfield Φ_{α} has fermionic and bosonic components, so that Eq. (2.20) should be replaced by

$$\begin{split} \partial_{\Lambda} \Gamma_{\Lambda}[\Phi] &= \\ \frac{1}{2} \mathrm{Tr} \left\{ \mathbf{Z} \left(\partial_{\Lambda} \mathbf{R}_{\Lambda} \right) \left[\left(\frac{\delta}{\delta \Phi} \otimes \frac{\delta}{\delta \Phi} \right)^{T} \Gamma_{\Lambda}[\Phi] + \mathbf{R}_{\Lambda} \right]^{-1} \right\}, \\ (4.15) \end{split}$$

where the matrix elements of the statistics matrix [3] are $[\mathbf{Z}]_{\alpha\beta} = \delta_{\alpha\beta}\zeta_{\alpha}$ with $\zeta_{\alpha} = 1$ if the label α corresponds to a Bose type X-operator, and $\zeta_{\alpha} = -1$ if α corresponds to a Fermi type X-operator. In analogy with Eq. (2.19), the regulator matrix \mathbf{R}_{Λ} is defined by writing the regulator term in Eq. (4.9) in (anti)-symmetrized superfield notation,

$$\int_{0}^{\beta} d\tau \sum_{ij\sigma} R_{ij,\Lambda}^{t} \left[\bar{X}_{i}^{\sigma 0}(\tau) \bar{X}_{j}^{0\sigma}(\tau) + \bar{X}_{i}^{2\bar{\sigma}}(\tau) \bar{X}_{j}^{\bar{\sigma}^{2}}(\tau) \right. \\
\left. + \bar{\sigma} \bar{X}_{i}^{\sigma 0}(\tau) \bar{X}_{j}^{\bar{\sigma}^{2}}(\tau) + \bar{\sigma} \bar{X}_{i}^{2\bar{\sigma}}(\tau) \bar{X}_{j}^{0\sigma}(\tau) \right] \\
= \frac{1}{2} \int_{\alpha} \int_{\alpha'} \Phi_{\alpha} [\mathbf{R}_{\Lambda}]_{\alpha\alpha'} \Phi_{\alpha'}. \tag{4.16}$$

Although the X-FRG Wetterich equation (4.15) is formally exact, in this form it is only of academic interest because in practice we have to impose the initial condition of decoupled sites where the deformed hopping $t_{ij,\Lambda=0}$ vanishes at the initial scale $\Lambda=0$. Unfortunately, in this limit the Legendre transform $\Gamma_{\Lambda=0}[\bar{X}]$ does not exist because for decoupled lattice sites the diagonal X-operators $X_i^{aa}(\tau)$ are constants of motion. This follows from the fact that in the interaction picture with respect to the single-site part $\mathcal{H}_1 = \sum_{ia} \epsilon_a X_i^{aa}$ of the Hamiltonian [see Eq. (3.17)] the X-operators satisfy the following equations of motion in imaginary time:

$$\frac{\partial X_i^{ab}(\tau)}{\partial \tau} = [\mathcal{H}_1, X_i^{ab}(\tau)] = (\epsilon_a - \epsilon_b) X_i^{ab}(\tau), \quad (4.17)$$

with the solution

$$X_i^{ab}(\tau) = e^{(\epsilon_a - \epsilon_b)\tau} X_i^{ab}(0). \tag{4.18}$$

Obviously, the diagonal operators $X_i^{aa}(\tau)$ are independent of τ ; moreover, in the absence of a magnetic field also the spin-flip operators $X_i^{\sigma\bar{\sigma}}(\tau)$ are conserved. The lack of intrinsic dynamics of some of the X-operators implies that the relations (4.10) cannot be inverted because the matrix of second derivatives of $\mathcal{G}_{\Lambda}[J]$ is not invertible at the initial scale $\Lambda=0$ where the hopping is switched off. A similar problem is encountered in the spin-FRG approach [7], where for vanishing exchange interactions the components of the individual spins parallel to the magnetic field do not have any dynamics. We can avoid

this problem by performing only a partial Legendre transform in the sector where the above second derivative matrix can be inverted. This can be implemented in two ways:

- 1. The simplest strategy is to include in the source term $\int_0^\beta d\tau \sum_{i,p} J_i^p(\tau) X_i^p(\tau)$ in Eq. (4.6) only those X-operators which have an intrinsic dynamics without hopping. The disadvantage of this approach is that correlation functions of the other X-operators are not easily accessible. If these fluctuations are singular, the resulting vertices of the X-operators which are retained are non-local so that simple approximations fail. Fortunately, for the Hubbard model all Fermi type X-operators do have intrinsic dynamics even for vanishing hopping, so that this strategy can be used to calculate the electronic single-particle spectral function of the Hubbard model. In fact, we will show in Sec. VA that this strategy reproduces the Hubbard-I approximation for the single-particle spectral function of the Hubbard model in a very simple way. Note also that there is a large degree of redundancy contained in the X-operators: for example, the Bose type Xoperator $X_i^{\sigma\sigma'}$ can be written as a composite operator involving a product of two Fermi type Xoperators, $X_i^{\sigma\sigma'} = X_i^{\sigma 0} X_i^{0\sigma'}$. Hence, even if we include only Fermi type X-operators in our Legendre transform, correlation functions of the Bose type X-operators can still be obtained as higher-order correlation functions of Fermi type X-operators.
- 2. To explicitly take into account also the fluctuations associated with the X-operators which do not have a dynamics for vanishing hopping, we can try to construct a suitable hybrid functional $\Phi_{\Lambda}[\bar{X}';\eta]$ which is defined via the usual Legendre transform with respect to all X-operators X' which do have intrinsic single-site dynamics, and includes the effect of the remaining set of X-operators via certain auxiliary fields η . For quantum spin systems we have explicitly constructed suitable hybrid functionals in our previous works 913. Although it is not clear how to generalize this strategy for the Hubbard model, for the t-J model this can be done in the same way as for quantum spin systems [9-13]. We will explicitly do this in the following subsection.

B. Flow equations for the t-J model

To derive the Wetterich equation for the t-J model we start again from Eq. (4.6) where it is now understood that the trace over the projected Hilbert space excludes states with doubly occupied sites and the sum $\sum_p J_i^p(\tau) X_i^p(\tau)$ in the source term is restricted to the nine X-operators acting on the projected Hilbert space. Instead of Eq. (4.8) we then obtain

$$\partial_{\Lambda} \mathcal{G}_{\Lambda}[J] = -\int_{0}^{\beta} d\tau \sum_{ij\sigma} (\partial_{\Lambda} t_{ij,\Lambda}) \left[\frac{\delta^{2} \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\sigma 0}(\tau) \delta J_{j}^{0\sigma}(\tau)} + \frac{\delta \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\sigma 0}(\tau)} \frac{\delta \mathcal{G}_{\Lambda}[J]}{\delta J_{j}^{0\sigma}(\tau)} \right]$$

$$-\frac{1}{4} \int_{0}^{\beta} d\tau \sum_{ij\sigma} (\partial_{\Lambda} J_{ij,\Lambda}) \left[\frac{\delta^{2} \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\sigma \overline{\sigma}}(\tau) \delta J_{j}^{\overline{\sigma}\sigma}(\tau)} + \frac{\delta \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\sigma \overline{\sigma}}(\tau)} \frac{\delta \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\overline{\sigma}\sigma}(\tau)} - \frac{\delta^{2} \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\sigma \overline{\sigma}}(\tau) \delta J_{j}^{\overline{\sigma}\overline{\sigma}}(\tau)} - \frac{\delta \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\sigma \overline{\sigma}}(\tau)} \frac{\delta \mathcal{G}_{\Lambda}[J]}{\delta J_{j}^{\overline{\sigma}\overline{\sigma}}(\tau)} \right].$$

$$(4.19)$$

The subtracted Legendre transform of $\mathcal{G}_{\Lambda}[J]$ is now defined by

$$\Gamma_{\Lambda}[\bar{X}] = \int_{0}^{\beta} d\tau \sum_{i,p} J_{i}^{p}(\tau) \bar{X}_{i}^{p}(\tau) - \mathcal{G}_{\Lambda}[J]
- \int_{0}^{\beta} d\tau \sum_{ij\sigma} \left\{ R_{ij,\Lambda}^{t} \bar{X}_{i}^{\sigma 0}(\tau) \bar{X}_{j}^{0\sigma}(\tau) + \frac{1}{4} R_{ij,\Lambda}^{J} \left[\bar{X}_{i}^{\sigma\bar{\sigma}}(\tau) \bar{X}_{j}^{\bar{\sigma}\sigma}(\tau) - \bar{X}_{i}^{\sigma\sigma}(\tau) \bar{X}_{j}^{\bar{\sigma}\bar{\sigma}}(\tau) \right] \right\},$$
(4.20)

which satisfies the flow equation

$$\begin{split} \partial_{\Lambda}\Gamma_{\Lambda}[\bar{X}] &= \int_{0}^{\beta} d\tau \sum_{ij\sigma} \Biggl\{ \left(\partial_{\Lambda} R_{ij,\Lambda}^{t} \right) \frac{\delta^{2} \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\sigma 0}(\tau) \delta J_{j}^{0\sigma}(\tau)} \\ &+ \frac{1}{4} \left(\partial_{\Lambda} R_{ij,\Lambda}^{J} \right) \Biggl[\frac{\delta^{2} \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\sigma \bar{\sigma}}(\tau) \delta J_{j}^{\bar{\sigma}\sigma}(\tau)} - \frac{\delta^{2} \mathcal{G}_{\Lambda}[J]}{\delta J_{i}^{\sigma \sigma}(\tau) \delta J_{j}^{\bar{\sigma}\bar{\sigma}}(\tau)} \Biggr] \Biggr\}. \end{split}$$

$$(4.21)$$

Finally, we introduce a nine-component superfield of the form (4.12); i.e.,

$$(\Phi_{\alpha}) = \begin{pmatrix} \Phi_{\uparrow} \\ \Phi_{\downarrow} \\ \Phi_{0} \\ \Phi_{2} \end{pmatrix}, \tag{4.22}$$

where now

$$\Phi_{\sigma} = \begin{pmatrix} \bar{X}^{0\sigma} \\ \bar{X}^{\sigma 0} \end{pmatrix}, \qquad \sigma = \uparrow, \downarrow, \tag{4.23}$$

and

$$\Phi_0 = \begin{pmatrix} \bar{X}^{\uparrow\uparrow} \\ \bar{X}^{\downarrow\downarrow} \\ \bar{X}^{\uparrow\downarrow} \\ \bar{X}^{\downarrow\uparrow} \end{pmatrix}, \qquad \Phi_2 = \bar{X}^{00}.$$
(4.24)

Defining the regulator matrix in superfield notation via

$$\int_{0}^{\beta} d\tau \sum_{ij\sigma} \left\{ R_{ij,\Lambda}^{t} \bar{X}_{i}^{\sigma 0}(\tau) \bar{X}_{j}^{0\sigma}(\tau) + \frac{1}{4} R_{ij,\Lambda}^{J} \left[\bar{X}_{i}^{\sigma \bar{\sigma}}(\tau) \bar{X}_{j}^{\bar{\sigma}\sigma}(\tau) - \bar{X}_{i}^{\sigma \sigma}(\tau) \bar{X}_{j}^{\bar{\sigma}\bar{\sigma}}(\tau) \right] \right\} \\
= \frac{1}{2} \int_{\alpha} \int_{\alpha'} \Phi_{\alpha} [\mathbf{R}_{\Lambda}]_{\alpha\alpha'} \Phi_{\alpha'}, \tag{4.25}$$

the resulting Wetterich equation for the t-J model is formally identical to the Wetterich equation for the Hubbard model given in Eq. (4.15). One should keep in mind, however, that for the t-J model the superfield Φ has only nine components and that the trace in Eq. (4.15) is over the projected Hilbert space of the t-J model.

As discussed at the end of Sec. $\overline{\text{IVA}}$ if we impose the initial condition $J_{ij,\Lambda=0}=0$ the Legendre transform $\Gamma_{\Lambda=0}[\bar{X}]$ defined in Eq. (4.20) does not exist because all X-operators of the Bose type are conserved for $\Lambda=0$. Let us now show how to solve this problem using the second method mentioned at the end of Sec. $\overline{\text{IVA}}$ therefore we introduce a hybrid functional $\Phi_{\Lambda}[\bar{\psi},\psi,\eta]$ which generates vertices that are propagator-irreducible with respect to the Fermi type X-operators, and in addition exchange interaction-irreducible with respect to the Bose type X-operators. For simplicity, we drop the particle-number term $\tilde{n}_j \tilde{n}_j/4$ in the t-J Hamiltonian and focus on the generating functional of connected correlation functions involving the four Fermi type X-operators $\tilde{c}_{i\sigma}^{\dagger} = X_i^{\sigma 0}$ and $\tilde{c}_{i\sigma} = X_i^{0\sigma}$ and on the three Bose type X-operators representing the spin components,

$$S_i^x = \frac{1}{2} \left(S_i^+ + S_i^- \right) = \frac{1}{2} \left(X_i^{+-} + X_i^{-+} \right),$$
 (4.26a)

$$S_i^y = \frac{1}{2i} \left(S_i^+ - S_i^- \right) = \frac{1}{2i} \left(X_i^{+-} - X_i^{-+} \right), \quad (4.26b)$$

$$S_i^z = \frac{1}{2} \left(X_i^{++} - X_i^{--} \right). \tag{4.26c}$$

The generating functional of the connected correlation functions of this set of X-operators can then be written as

$$e^{\mathcal{G}_{\Lambda}[\vec{j},j,\boldsymbol{h}]} = \operatorname{Tr}\left\{e^{-\beta\mathcal{H}_{1}}\mathcal{T}e^{-\int_{0}^{\beta}d\tau\mathcal{H}_{2,\Lambda}(\tau)}e^{\int_{0}^{\beta}d\tau\sum_{i\sigma}\left[\vec{j}_{i\sigma}(\tau)\tilde{c}_{i\sigma}(\tau)+\tilde{c}_{i\sigma}^{\dagger}(\tau)j_{i\sigma}(\tau)\right]}e^{\int_{0}^{\beta}d\tau\sum_{i}\boldsymbol{h}_{i}(\tau)\cdot\boldsymbol{S}_{i}(\tau)}\right\},\tag{4.27}$$

where $\mathcal{H}_1 = -\mu \sum_{i\sigma} X_i^{\sigma\sigma}$ and

$$\mathcal{H}_{2,\Lambda} = \sum_{ij\sigma} t_{ij,\Lambda} \tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{j\sigma} + \frac{1}{2} \sum_{ij} J_{ij,\Lambda} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{4.28}$$

The generating functional of connected correlation functions of Fermi type X-operators and interaction-amputated spin correlation functions is [7] [9]

$$\mathcal{F}_{\Lambda}[\bar{j}, j, \boldsymbol{m}] = \mathcal{G}_{\Lambda}[\bar{j}, j, \boldsymbol{h} \to -\sum_{j} J_{ij,\Lambda} \boldsymbol{m}_{j}] - \frac{1}{2} \int_{0}^{\beta} d\tau \sum_{ij} J_{ij,\Lambda} \boldsymbol{m}_{i}(\tau) \cdot \boldsymbol{m}_{j}(\tau). \tag{4.29}$$

This functional satisfies the flow equation [7],

$$\partial_{\Lambda} \mathcal{F}_{\Lambda}[\bar{j}, j, \boldsymbol{m}] = -\zeta \int_{0}^{\beta} d\tau \sum_{ij\sigma} \left(\partial_{\Lambda} t_{ij,\Lambda} \right) \left[\frac{\delta^{2} \mathcal{F}_{\Lambda}[\bar{j}, j, \boldsymbol{m}]}{\delta j_{i\sigma}(\tau) \delta \bar{j}_{j\sigma}(\tau)} + \frac{\delta \mathcal{F}_{\Lambda}[\bar{j}, j, \boldsymbol{m}]}{\delta j_{i\sigma}(\tau)} \frac{\delta \mathcal{F}_{\Lambda}[\bar{j}, j, \boldsymbol{m}]}{\delta \bar{j}_{j\sigma}(\tau)} \right]$$

$$+ \frac{1}{2} \int_{0}^{\beta} d\tau \sum_{ij\alpha} \left(\partial_{\Lambda} \mathbb{J}_{\Lambda}^{-1} \right)_{ij} \left[\frac{\delta^{2} \mathcal{F}_{\Lambda}[\bar{j}, j, \boldsymbol{m}]}{\delta m_{i}^{\alpha}(\tau) \delta m_{j}^{\alpha}(\tau)} + \frac{\delta \mathcal{F}_{\Lambda}[\bar{j}, j, \boldsymbol{m}]}{\delta m_{i}^{\alpha}(\tau)} \frac{\delta \mathcal{F}_{\Lambda}[\bar{j}, j, \boldsymbol{m}]}{\delta m_{j}^{\alpha}(\tau)} \right] + \frac{1}{2} \operatorname{Tr} \left[\mathbf{J}_{\Lambda} \partial_{\Lambda} \mathbf{J}_{\Lambda}^{-1} \right], \quad (4.30)$$

where \mathbb{J}_{Λ} is a matrix in the site labels i, j with matrix elements $[\mathbb{J}_{\Lambda}]_{ij} = J_{ij,\Lambda}$ and \mathbf{J} is a matrix in the site (i), imaginary time (τ) , and spin component (α) labels with matrix elements

$$[\mathbf{J}_{\Lambda}]_{i\tau\alpha,j\tau'\alpha'} = J_{ij,\Lambda}\delta_{\alpha\alpha'}\delta(\tau - \tau'). \tag{4.31}$$

The generating functional of vertices which are propagator-irreducible for the Fermi type fields and exchange-interaction irreducible for the Bose type fields is now defined via the following subtracted Legendre transform,

$$\Gamma_{\Lambda}[\bar{\psi}, \psi, \boldsymbol{\eta}] = \int_{0}^{\beta} d\tau \sum_{i\sigma} \left[\bar{j}_{i\sigma}(\tau) \psi_{i\sigma}(\tau) + \bar{\psi}_{i\sigma}(\tau) j_{i\sigma}(\tau) \right] + \int_{0}^{\beta} d\tau \sum_{i} \boldsymbol{m}_{i}(\tau) \cdot \boldsymbol{\eta}_{i}(\tau) - \mathcal{F}_{\Lambda}[\bar{j}, j, \boldsymbol{m}]$$

$$- \int_{0}^{\beta} d\tau \sum_{ij\sigma} t_{ij,\Lambda} \bar{\psi}_{i\sigma}(\tau) \psi_{j\sigma}(\tau) + \frac{1}{2} \int_{0}^{\beta} d\tau \sum_{ij} [\mathbb{J}_{\Lambda}^{-1}]_{ij} \boldsymbol{\eta}_{i}(\tau) \cdot \boldsymbol{\eta}_{j}(\tau),$$

$$(4.32)$$

where

$$\psi_{i\sigma}(\tau) = \langle \mathcal{T}\tilde{c}_{i\sigma}(\tau) \rangle = \frac{\delta \mathcal{F}_{\Lambda}[\bar{j}, j, \mathbf{m}]}{\delta \bar{j}_{i\sigma}(\tau)}, \tag{4.33a}$$

$$\bar{\psi}_{i\sigma}(\tau) = \langle \mathcal{T}\hat{c}_{i\sigma}^{\dagger}(\tau) \rangle = \zeta \frac{\delta \mathcal{F}_{\Lambda}[\bar{j}, j, m]}{\delta i_{i\sigma}(\tau)}, \tag{4.33b}$$

$$\eta_i(\tau) = \frac{\delta \mathcal{F}_{\Lambda}[\bar{j}, j, m]}{\delta m_i(\tau)}.$$
(4.33c)

By construction, the functional $\Gamma_{\Lambda}[\bar{\psi}, \psi, \eta]$ satisfies the flow equation

$$\partial_{\Lambda}\Gamma_{\Lambda}[\bar{\psi},\psi,\boldsymbol{\eta}] = \zeta \int_{0}^{\beta} d\tau \sum_{ij\sigma} \left(\partial_{\Lambda}t_{ij,\Lambda}\right) \frac{\delta^{2}\mathcal{F}_{\Lambda}[\bar{j},j,\boldsymbol{m}]}{\delta j_{i\sigma}(\tau)\delta \bar{j}_{j\sigma}(\tau)} - \frac{1}{2} \int_{0}^{\beta} d\tau \sum_{ij\alpha} \left(\partial_{\Lambda}\mathbb{J}_{\Lambda}^{-1}\right)_{ij} \frac{\delta^{2}\mathcal{F}_{\Lambda}[\bar{j},j,\boldsymbol{m}]}{\delta m_{i}^{\alpha}(\tau)\delta m_{j}^{\alpha}(\tau)} - \frac{1}{2} \operatorname{Tr}\left[\mathbf{J}_{\Lambda}\partial_{\Lambda}\mathbf{J}_{\Lambda}^{-1}\right].$$

The right-hand side of this flow equation has a finite limit for vanishing exchange couplings. To see this more clearly, let us for simplicity set $t_{ij,\Lambda} = 0$ and focus only on the flow in the spin sector, which can be derived from the functional $\Phi_{\Lambda}[\boldsymbol{\eta}] = \Gamma_{\Lambda}[0,0,\boldsymbol{\eta}]$. It satisfies the flow equation

$$\partial_{\Lambda}\Phi_{\Lambda}[\boldsymbol{\eta}] = -\frac{1}{2}\operatorname{Tr}\left\{\left[\left(\boldsymbol{\Phi}_{\Lambda}^{"}[\boldsymbol{\eta}] - \mathbf{J}_{\Lambda}^{-1}\right)^{-1} + \mathbf{J}_{\Lambda}\right]\partial_{\Lambda}\mathbf{J}_{\Lambda}^{-1}\right\} = -\frac{1}{2}\operatorname{Tr}\left\{\boldsymbol{\Phi}_{\Lambda}^{"}[\boldsymbol{\eta}]\left(\mathbf{1} - \mathbf{J}_{\Lambda}\boldsymbol{\Phi}_{\Lambda}^{"}[\boldsymbol{\eta}]\right)^{-1}\partial_{\Lambda}\mathbf{J}_{\Lambda}\right\},\tag{4.35}$$

where Φ''_{Λ} denotes the matrix of second derivatives with respect to the components of the η -field,

$$\left[\mathbf{\Phi}_{\Lambda}^{"}[\boldsymbol{\eta}]\right]_{i\tau\alpha,j\tau'\alpha'} = \frac{\delta^{2}\Phi_{\Lambda}[\boldsymbol{\eta}]}{\delta\eta_{i}^{\alpha}(\tau)\delta\eta_{j}^{\alpha'}(\tau')}.$$
(4.36)

From the right-hand side of Eq. (4.35), it is obvious that the functional $\Phi_{\Lambda}[\eta]$ is well-defined even for $\mathbf{J}_{\Lambda} = 0$. The second functional derivatives on the right-hand side of Eq. (4.34) can be expressed in terms of the second derivatives of $\Gamma_{\Lambda}[\bar{\psi}, \psi, \eta]$. At this point, it is convenient to use again a superfield notation with a seven-component superfield

$$(\Phi_{\alpha}) = \begin{pmatrix} \psi_{\uparrow} \\ \bar{\psi}_{\uparrow} \\ \psi_{\downarrow} \\ \bar{\psi}_{\downarrow} \end{pmatrix}. \tag{4.37}$$

Then the flow equation (4.34) can be cast into the form

$$\partial_{\Lambda} \Gamma_{\Lambda}[\Phi] = \frac{1}{2} \operatorname{Tr} \left\{ \mathbf{Z} \left(\partial_{\Lambda} \mathbf{T}_{\Lambda} \right) \left[\left(\frac{\delta}{\delta \Phi} \otimes \frac{\delta}{\delta \Phi} \right)^{T} \Gamma_{\Lambda}[\Phi] + \mathbf{T}_{\Lambda} \right]^{-1} \right\} - \frac{1}{2} \operatorname{Tr} \left[\mathbf{J}_{\Lambda} \partial_{\Lambda} \mathbf{J}_{\Lambda}^{-1} \right], \tag{4.38}$$

where the generalized hopping matrix T_{Λ} in superfield space is defined by writing

$$\int_{0}^{\beta} d\tau \sum_{ij\sigma} t_{ij,\Lambda} \bar{\psi}_{i\sigma}(\tau) \psi_{j\sigma}(\tau) - \frac{1}{2} \int_{0}^{\beta} d\tau \sum_{ij} [\mathbb{J}_{\Lambda}^{-1}]_{ij} \eta_{i}(\tau) \cdot \eta_{j}(\tau) = \frac{1}{2} \int_{\alpha} \int_{\alpha'} \Phi_{\alpha}[\mathbf{T}_{\Lambda}]_{\alpha\alpha'} \Phi_{\alpha'}. \tag{4.39}$$

The functional $\Gamma_{\Lambda}[\Phi]$ is well-defined for all Λ , including $\Lambda = 0$ where both hopping and the exchange interaction vanish.

V. SIMPLE APPLICATIONS

A. Hubbard-I approximation from X-FRG

If we are only interested in correlation functions of the Fermi type X-operators (which is sufficient for the calcu-

lation of the single-particle Green function of the Hubbard model), we may solve the initial value problem by including only the Fermi type X-operators in the source term $\int_0^\beta d\tau \sum_{i,p} J_i^p(\tau) X_i^p(\tau)$ in the definition (4.6) of the generating functional $G_{\Lambda}[J]$; see the first strategy discussed in Sec. IVA after Eq. (4.18). Up to quadratic order in the expectation values $X^{ab} = \langle X^{ab} \rangle$ of the X-operators the generating functional $\Gamma_{\Lambda}[\bar{X}]$ of the irreducible X-operator vertices defined in Eq. (4.9) has the following expansion in momentum-frequency space:

$$\Gamma_{\Lambda}[\bar{X}] = \Gamma_{\Lambda}[0] + \int_{K} \sum_{\sigma} \left\{ \left[t_{k} + \Sigma_{\Lambda}^{\sigma0,0\sigma}(K) \right] \bar{X}_{-K}^{\sigma0} \bar{X}_{K}^{0\sigma} + \left[t_{k} + \Sigma_{\Lambda}^{2\bar{\sigma},\bar{\sigma}^{2}}(K) \right] \bar{X}_{-K}^{2\bar{\sigma}} \bar{X}_{K}^{\bar{\sigma}^{2}} \right. \\
\left. + \bar{\sigma} \left[t_{k} + \Sigma_{\Lambda}^{\sigma0,\bar{\sigma}^{2}}(K) \right] \bar{X}_{-K}^{\sigma0} \bar{X}_{K}^{\bar{\sigma}^{2}} + \bar{\sigma} \left[t_{k} + \Sigma_{\Lambda}^{2\bar{\sigma},0\sigma}(K) \right] \bar{X}_{-K}^{2\bar{\sigma}} \bar{X}_{K}^{0\sigma} \right\} + \dots \\
= \Gamma_{\Lambda}[0] + \int_{K} \sum_{\sigma} \psi_{K\sigma}^{\dagger} \left(t_{k} + \Sigma_{\Lambda}^{\sigma0,0\sigma}(K) \ t_{k} + \Sigma_{\Lambda}^{\sigma0,\bar{\sigma}^{2}}(K) \right) \psi_{K\sigma} + \dots , \tag{5.1}$$

where the collective label $K=(\boldsymbol{k},\omega)$ denotes momentum and fermionic Matsubara frequency, the integration symbol is defined as $\int_K = \frac{1}{\beta N} \sum_{\boldsymbol{k}\omega}$, where N is the number of lattice sites, and the Fourier expansions of the expectation values of the X-operators and the hopping are

defined by

$$\bar{X}_{i}^{ab}(\tau) = \frac{1}{\beta N} \sum_{\mathbf{k},\omega} e^{i(\mathbf{k}\cdot\mathbf{r}_{i}-\omega\tau)} \bar{X}_{K}^{ab}, \tag{5.2}$$

$$t_{ij} = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} t_{\mathbf{k}}.$$
 (5.3)

In the second line of Eq. (5.1), we have introduced two-component vectors analogous to Eq. (3.12),

$$\psi_{K\sigma} = \begin{pmatrix} \bar{X}_K^{0\sigma} \\ \bar{\sigma}\bar{X}_K^{\bar{\sigma}2} \end{pmatrix}, \quad \psi_{K\sigma}^{\dagger} = (\bar{X}_{-K}^{\sigma 0}, \bar{\sigma}\bar{X}_{-K}^{2\bar{\sigma}}). \tag{5.4}$$

For a given value of the deformation parameter Λ the deformed two-point functions of the Fermi type X-operators are

$$\begin{pmatrix}
G_{\Lambda}^{\sigma0,0\sigma}(K) & \bar{\sigma}G_{\Lambda}^{\sigma0,\bar{\sigma}2}(K) \\
\bar{\sigma}G_{\Lambda}^{2\bar{\sigma},0\sigma}(K) & G_{\Lambda}^{2\bar{\sigma},\bar{\sigma}2}(K)
\end{pmatrix} = \\
- \begin{pmatrix}
t_{\mathbf{k},\Lambda} + \Sigma_{\Lambda}^{\sigma0,0\sigma}(K) & t_{\mathbf{k},\Lambda} + \Sigma_{\Lambda}^{\sigma0,\bar{\sigma}2}(K) \\
t_{\mathbf{k},\Lambda} + \Sigma_{\Lambda}^{2\bar{\sigma},0\sigma}(K) & t_{\mathbf{k},\Lambda} + \Sigma_{\Lambda}^{2\bar{\sigma},\bar{\sigma}2}(K)
\end{pmatrix}^{-1} = \\
\frac{-1}{D_{\Lambda}(K)} \begin{pmatrix}
t_{\mathbf{k},\Lambda} + \Sigma_{\Lambda}^{2\bar{\sigma},\bar{\sigma}2}(K) & -t_{\mathbf{k},\Lambda} - \Sigma_{\Lambda}^{\sigma0,\bar{\sigma}2}(K) \\
-t_{\mathbf{k},\Lambda} - \Sigma_{\Lambda}^{2\bar{\sigma},0\sigma}(K) & t_{\mathbf{k},\Lambda} + \Sigma_{\Lambda}^{\sigma0,0\sigma}(K)
\end{pmatrix}, (5.5)$$

where $t_{\mathbf{k},\Lambda} = t_{\mathbf{k}} + R_{\mathbf{k},\Lambda}^t$ is the Fourier transform of the deformed hopping and

$$D_{\Lambda}(K) = \left[t_{\mathbf{k},\Lambda} + \Sigma_{\Lambda}^{\sigma 0,0\sigma}(K) \right] \left[t_{\mathbf{k},\Lambda} + \Sigma_{\Lambda}^{2\bar{\sigma},\bar{\sigma}2}(K) \right] - \left[t_{\mathbf{k},\Lambda} + \Sigma_{\Lambda}^{\sigma 0,\bar{\sigma}2}(K) \right] \left[t_{\mathbf{k},\Lambda} + \Sigma_{\Lambda}^{2\bar{\sigma},0\sigma}(K) \right].$$

$$(5.6)$$

With the initial condition $t_{k,\Lambda=0} = 0$, the initial self-energies are given by the inverse two-point functions of the X-operators in the atomic limit. A general method for calculating arbitrary correlation functions of X-operators in the atomic limit is presented in Appendix A In Appendix B we summarize the result for the two-point function. Using Eq. (B39), we obtain

$$\begin{pmatrix} \Sigma_0^{\sigma0,0\sigma}(K) & \Sigma_0^{\sigma0,\bar{\sigma}2}(K) \\ \Sigma_0^{2\bar{\sigma},0\sigma}(K) & \Sigma_0^{2\bar{\sigma},\bar{\sigma}2}(K) \end{pmatrix} = \begin{pmatrix} -\frac{i\omega+\mu}{x_0+x_\sigma} & 0 \\ 0 & -\frac{i\omega+\mu-U}{x_2+x_{\bar{\sigma}}} \end{pmatrix}, \tag{5.7}$$

where

$$x_a = \langle X_i^{aa} \rangle, \qquad a = 0, \uparrow, \downarrow, 2,$$
 (5.8)

are the expectation values of the diagonal X-operators in the atomic limit. The Hubbard-I approximation amounts to replacing the flowing self-energies of the X-operators by their initial values given in Eq. (5.7). In this approximation, the X-operator two-point functions are for $\Lambda \to 1$ (where $t_{\boldsymbol{k},\Lambda} \to t_{\boldsymbol{k}}$) given by

$$\begin{pmatrix}
G^{\sigma 0,0\sigma}(K) & \bar{\sigma}G^{\sigma 0,\bar{\sigma}^{2}}(K) \\
\bar{\sigma}G^{2\bar{\sigma},0\sigma}(K) & G^{2\bar{\sigma},\bar{\sigma}^{2}}(K)
\end{pmatrix}$$

$$= \frac{1}{D(K)} \begin{pmatrix}
\frac{i\omega + \mu - U}{x_{2} + x_{\bar{\sigma}}} - t_{\mathbf{k}} & t_{\mathbf{k}} \\
t_{\mathbf{k}} & \frac{i\omega + \mu}{x_{0} + x_{\sigma}} - t_{\mathbf{k}}
\end{pmatrix}, (5.9)$$

with

$$D(K) = \left[\frac{i\omega + \mu}{x_0 + x_\sigma} - t_{\mathbf{k}} \right] \left[\frac{i\omega + \mu - U}{x_2 + x_{\bar{\sigma}}} - t_{\mathbf{k}} \right] - t_{\mathbf{k}}^2$$

$$= \left[\frac{i\omega + \mu}{x_0 + x_\sigma} \right] \left[\frac{i\omega + \mu - U}{x_2 + x_{\bar{\sigma}}} \right]$$

$$- t_{\mathbf{k}} \left[\frac{i\omega + \mu}{x_0 + x_\sigma} + \frac{i\omega + \mu - U}{x_2 + x_{\bar{\sigma}}} \right]. \tag{5.10}$$

The corresponding electronic Green function for spin σ electrons is

$$G_{\sigma}(K) = G^{0\sigma,\sigma0}(K) + G^{\bar{\sigma}2,2\bar{\sigma}}(K)$$

$$+ \bar{\sigma}G^{0\sigma,2\bar{\sigma}}(K) + \bar{\sigma}G^{\bar{\sigma}2,\sigma0}(K)$$

$$= \frac{\frac{i\omega+\mu}{x_0+x_{\sigma}} + \frac{i\omega+\mu-U}{x_2+x_{\bar{\sigma}}}}{\left[\frac{i\omega+\mu}{x_0+x_{\sigma}}\right]\left[\frac{i\omega+\mu-U}{x_2+x_{\bar{\sigma}}}\right] - t_{\mathbf{k}}\left[\frac{i\omega+\mu}{x_0+x_{\sigma}} + \frac{i\omega+\mu-U}{x_2+x_{\bar{\sigma}}}\right]}$$

$$= \frac{\frac{x_0+x_{\sigma}}{i\omega+\mu} + \frac{x_2+x_{\bar{\sigma}}}{i\omega+\mu-U}}{1 - t_{\mathbf{k}}\left[\frac{x_0+x_{\sigma}}{i\omega+\mu} + \frac{x_2+x_{\bar{\sigma}}}{i\omega+\mu-U}\right]}.$$
(5.11)

Keeping in mind that in the atomic limit the probability of finding an electron with spin σ is $n_{\sigma} = x_2 + x_{\sigma}$ and using

$$x_0 + x_{\sigma} = 1 - (x_{\uparrow} + x_{\downarrow} + x_2) + x_{\sigma}$$

= 1 - x_2 - x_{\bar{\sigma}} = 1 - n_{\bar{\sigma}}, \tag{(5.12)}

we see that $G_{\sigma}(K)$ in Eq. (5.11) can also be written as

$$G_{\sigma}(K)$$

$$= \frac{i\omega + \mu - U(1 - n_{\bar{\sigma}})}{(i\omega + \mu)(i\omega + \mu - U) - t_{\mathbf{k}}[i\omega + \mu - U(1 - n_{\bar{\sigma}})]}$$
$$= \frac{i\omega + \mu - U(1 - n_{\bar{\sigma}})}{(i\omega + \mu - \epsilon_{\mathbf{k}}^{+})(i\omega + \mu - \epsilon_{\mathbf{k}}^{-})}, \tag{5.13}$$

where

$$\epsilon_{\mathbf{k}}^{\pm} = \frac{t_{\mathbf{k}} + U}{2} \pm \sqrt{\left(\frac{t_{\mathbf{k}} - U}{2}\right)^2 + t_{\mathbf{k}} U n_{\bar{\sigma}}}.$$
 (5.14)

Equation (5.13) is the well-known Hubbard-I approximation for the electronic single-particle Green functions of the Hubbard model [15], [20], which is exact both in the non-interacting limit $U \to 0$ and in the atomic limit $t_k \to 0$. Note that for vanishing magnetic field $n_{\uparrow} = n_{\downarrow}$ is independent of the spin projection σ . From Eq. (5.13) it is clear, that the X-operator self-energies defined in Eq. (5.7) are non-trivially related to the usual self-energy $\Sigma(K)$ defined via $G_{\sigma}^{-1}(K) = i\omega + \mu - t_k - \Sigma(K)$. Therefore even the initial condition of our X-FRG approach amounts to a non-trivial resummation in perturbation theory.

B. Quasi-particles in the hidden Fermi liquid

In this section, we focus on the Hubbard model for infinite on-site repulsion, i.e. the t model introduced in

Sec. IIIC The Hamiltonian of the model consists only of the projected kinetic energy given in Eq. (3.31). A slight complication arises from the fact that for fixed electronic filling n the chemical potential μ_{Λ} depends on the flow-parameter Λ when the hopping is switched on. In a conventional Fermi liquid one usually eliminates the associated shift in the self-energy via a suitable counter term [31]. To implement a similar procedure in our FRG approach to the t model, we use the operator identity $X_i^{\sigma 0} X_i^{0\sigma} = X_i^{\sigma \sigma}$ to rewrite the deformed grand canonical Hamiltonian of the t model as

$$\tilde{\mathcal{H}}_{t,\Lambda} = \mathcal{H}_1 + \mathcal{H}_{2,\Lambda},\tag{5.15}$$

with

$$\mathcal{H}_1 = -\mu_0 \sum_{i\sigma} \tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{i\sigma} = -\mu_0 \sum_{i\sigma} X_i^{\sigma\sigma}, \qquad (5.16)$$

$$\mathcal{H}_{2,\Lambda} = \sum_{ij\sigma} (t_{ij,\Lambda} - \delta\mu_{\Lambda}) \,\tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{j\sigma}, \qquad (5.17)$$

where

$$\delta\mu_{\Lambda} = \mu_{\Lambda} - \mu_0 \tag{5.18}$$

is the difference between the chemical potential μ_{Λ} at scale Λ and the chemical potential μ_0 in the atomic limit (i.e., for vanishing hopping), which for a given electronic filling n_0 is determined by the atomic equation of state,

$$n_0 = \frac{2e^{\beta\mu_0}}{1 + 2e^{\beta\mu_0}}. (5.19)$$

Solving for μ_0 we obtain

$$\mu_0 = T \ln \left(\frac{n_0}{2(1 - n_0)} \right). \tag{5.20}$$

Assuming that at the initial value $\Lambda=0$ the deformed hopping $t_{ij,\Lambda=0}$ vanishes, the initial generating functional of the connected correlation functions is

$$e^{\mathcal{G}_0[J]} = \operatorname{Tr}\left[e^{-\beta\mathcal{H}_1}\mathcal{T}e^{\int_0^\beta d\tau \sum_{i,p} J_i^p(\tau)X_i^p(\tau)}\right].$$
 (5.21)

Since the sites are decoupled in this limit, the generating functional is the sum of single-site generating functionals,

$$\mathcal{G}_0[J] = \sum_i \mathcal{G}_{\text{site}}[J_i], \qquad (5.22)$$

where the generating functional of the single-site (atomic) correlation functions is

$$\mathcal{G}_{\text{site}}[J] = \ln \operatorname{tr} \left[e^{\beta \mu_0 \sum_{\sigma} X^{\sigma \sigma}} \mathcal{T} e^{\int_0^{\beta} d\tau \sum_{p} J^p(\tau) X^p(\tau)} \right].$$
(5.23)

Here, the symbol tr[...] denotes the trace over the threestate projected Hilbert space associated with a single lattice site. Since we are only interested in the correlation functions of the Fermi type X-operators, it is sufficient to introduce only four Grassmann sources $J^{0\uparrow}$, $J^{\uparrow 0}$, $J^{0\downarrow}$ and $J^{\downarrow 0}$. The source term then reduces to

$$\int_{0}^{\beta} d\tau \sum_{p} J^{p}(\tau) X^{p}(\tau)$$

$$= \int_{0}^{\beta} \sum_{\sigma} \left[J^{0\sigma}(\tau) X^{0\sigma}(\tau) + J^{\sigma 0}(\tau) X^{\sigma 0}(\tau) \right]$$

$$= \int_{0}^{\beta} d\tau \sum_{\sigma} \left[J^{0\sigma}(\tau) \tilde{c}_{\sigma}(\tau) + J^{\sigma 0}(\tau) \tilde{c}_{\sigma}^{\dagger}(\tau) \right]$$

$$= \int_{0}^{\beta} d\tau \sum_{\sigma} \left[\bar{j}_{\sigma}(\tau) \tilde{c}_{\sigma}(\tau) + \tilde{c}_{\sigma}^{\dagger}(\tau) j_{\sigma}(\tau) \right], \qquad (5.24)$$

where in the last line we have set $J^{0\sigma}(\tau) = \bar{j}_{\sigma}(\tau)$ and $J^{\sigma 0}(\tau) = \zeta j_{\sigma}(\tau) = -j_{\sigma}(\tau)$. With the notation

$$\psi_{i\sigma} = \bar{X}_i^{0\sigma} = \langle \tilde{c}_{i\sigma} \rangle, \quad \bar{\psi}_{i\sigma} = \bar{X}_i^{\sigma 0} = \langle \tilde{c}_{i\sigma}^{\dagger} \rangle, \quad (5.25)$$

the generating functional $\Gamma_{\Lambda}[\bar{\psi}, \psi] = \Gamma_{\Lambda}[\bar{X}]$ defined in Eq. (4.20) has for the t model the following vertex expansion in momentum-frequency space:

$$\Gamma_{\Lambda}[\bar{\psi}, \psi] = \Gamma_{\Lambda}[0, 0] + \int_{K} \sum_{\sigma} [t_{k} + \Sigma_{\Lambda}(K)] \bar{\psi}_{K\sigma} \psi_{K\sigma}$$

$$+ \frac{1}{(2!)^{2}} \int_{K'_{1}} \int_{K'_{2}} \int_{K_{2}} \int_{K_{1}} \sum_{\sigma'_{1}\sigma'_{2}\sigma_{2}\sigma_{1}} \delta_{K'_{1}+K'_{2},K_{2}+K_{1}}$$

$$\times \Gamma_{\Lambda}^{\bar{\psi}\bar{\psi}\psi} (K'_{1}\sigma'_{1}, K'_{2}\sigma'_{2}; K_{2}\sigma_{2}, K_{1}\sigma_{1})$$

$$\times \bar{\psi}_{K'_{1}\sigma'_{1}} \bar{\psi}_{K'_{2}\sigma'_{2}} \psi_{K_{2}\sigma_{2}} \psi_{K_{1}\sigma_{1}} + \dots ,$$
 (5.26)

where $\delta_{K,0} = \beta N \delta_{k,0} \delta_{\omega,0}$ and the ellipsis denotes higher-order vertices. The Fourier components are defined as

$$\psi_{K\sigma} = \bar{X}_K^{0\sigma} = \sum_i \int_0^\beta d\tau e^{-i(\mathbf{k}\cdot\mathbf{r}_i - \omega\tau)} \psi_{i\sigma}(\tau), \quad (5.27a)$$

$$\bar{\psi}_{K\sigma} = \bar{X}_{-K}^{\sigma 0} = \sum_{i} \int_{0}^{\beta} d\tau e^{i(\mathbf{k}\cdot\mathbf{r}_{i} - \omega\tau)} \bar{\psi}_{i\sigma}(\tau). \quad (5.27b)$$

The scale-dependent irreducible four-point vertex in Eq. (5.26) is antisymmetric with respect to the exchange of the first two outgoing labels $K'_1\sigma'_1 \leftrightarrow K'_2\sigma'_2$ and with respect to the exchange of the two incoming labels $K_1\sigma_1 \leftrightarrow K_2\sigma_2$. Note that the SU(2) spin-rotational invariance of the Hubbard model implies that the spin-dependence of the antisymmetrized effective interaction is of the form 3

$$\Gamma_{\Lambda}^{\bar{\psi}\bar{\psi}\psi\psi}(K'_{1}\sigma'_{1}, K'_{2}\sigma'_{2}; K_{2}\sigma_{2}, K_{1}\sigma_{1})$$

$$= \delta_{\sigma'_{1}\sigma_{1}}\delta_{\sigma'_{2}\sigma_{2}}U_{\Lambda}(K'_{1}, K'_{2}; K_{2}, K_{1})$$

$$- \delta_{\sigma'_{1}\sigma_{2}}\delta_{\sigma'_{2}\sigma_{1}}U_{\Lambda}(K'_{1}, K'_{2}; K_{1}, K_{2}), \qquad (5.28)$$

where the function $U_{\Lambda}(K'_1, K'_2; K_1, K_2)$ is symmetric under the simultaneous exchange of its outgoing and incoming labels,

$$U_{\Lambda}(K_1', K_2'; K_2, K_1) = U_{\Lambda}(K_2', K_1'; K_1, K_2). \tag{5.29}$$

An alternative parametrization of the vertex expansion (5.26) is therefore

$$\Gamma_{\Lambda}[\bar{\psi}, \psi] = \Gamma_{\Lambda}[0, 0] + \int_{K} \sum_{\sigma} [t_{k} + \Sigma_{\Lambda}(K)] \bar{\psi}_{K\sigma} \psi_{K\sigma}
+ \frac{1}{2} \int_{K'_{1}} \int_{K'_{2}} \int_{K_{2}} \int_{K_{1}} \sum_{\sigma_{1}\sigma_{2}} \delta_{K'_{1} + K'_{2}, K_{2} + K_{1}}
\times U_{\Lambda}(K'_{1}, K'_{2}; K_{2}, K_{1}) \bar{\psi}_{K'_{1}\sigma_{1}} \bar{\psi}_{K'_{2}\sigma_{2}} \psi_{K_{2}\sigma_{2}} \psi_{K_{1}\sigma_{1}}
+ \dots$$
(5.30)

It is important to emphasize that the four-point vertex and the higher-order vertices represented by the ellipsis in the vertex expansions (5.26) and (5.30) arise from the kinematic correlations due to the Hilbert space projection in the t model model. If we replace the projected Fermilike operators \tilde{c}_{σ} and $\tilde{c}_{\sigma}^{\dagger}$ by canonical fermions and thus neglect the Hilbert space projection, the generating functional $\mathcal{G}_{\text{site}}[J]$ reduces to a trivial quadratic functional of the sources, so that all interaction vertices in the vertex expansion (5.26) vanish and the self-energy $\Sigma_{\Lambda}(K)$ reduces to $-i\omega - \mu$.

For a given value of Λ , the deformed two-point function of the projected fermions is

$$G_{\Lambda}(\mathbf{k},\omega) = \frac{-1}{t_{\mathbf{k},\Lambda} - \delta\mu_{\Lambda} + \Sigma_{\Lambda}(\mathbf{k},\omega)},$$
 (5.31)

where the initial value of the self-energy is given by its atomic limit derived in Appendix B

$$\Sigma_0(\omega) = -\frac{i\omega + \mu_0}{1 - \frac{n_0}{2}}.$$
 (5.32)

Following the usual procedure [31], we assume that the counter-term $\delta\mu_{\Lambda}$ takes the shift in the chemical potential due to the self-energy at zero frequency into account. Thus, we demand that

$$\Sigma_{\Lambda}(\mathbf{k}_F, 0) = \Sigma_0(\omega = 0) = -\frac{\mu_0}{1 - \frac{n_0}{2}}.$$
 (5.33)

for wavevectors k_F on the Fermi surface. As $\mu_0 \to 0$ for $T \to 0$ according to Eq. (5.20), the flowing Fermi surface is then determined by

$$t_{\mathbf{k}_F,\Lambda} = \delta\mu_{\Lambda} = \mu_{\Lambda} \tag{5.34}$$

at zero temperature. Actually, as pointed out by Anderson [31], in general the counter-term $\delta\mu$ depends on the momentum k_F on the Fermi surface. Here we can ignore this subtlety because within our truncation the self-energy $\Sigma_{\Lambda}(\omega)$ is momentum-independent. Once we have determined the two-point function [5.31] within some approximation, we can obtain the equation of state at a given Λ in the implicit form

$$n_{\Lambda} = \frac{2}{\beta N} \sum_{\mathbf{k}, \omega} G_{\Lambda}(\mathbf{k}, \omega) e^{i\omega 0^{+}}, \qquad (5.35)$$

where the right-hand side depends on μ_{Λ} and n_{Λ} .

Before investigating the actual flow equations, it is instructive to consider the approximation where the self-energy $\Sigma_{\Lambda}(\omega)$ is replaced by its atomic limit (5.32). In this case the above counter-term procedure is not directly applicable because the condition (5.33) is trivially fulfilled. Therefore we fix the counter-term $\delta\mu_{\Lambda}$ instead by demanding that the filling does not change during the flow; i.e., $n_{\Lambda} = n_0 = n$. For a given filling n, the bare chemical potential $\mu_0 = \mu_0(n,T)$ is then given by Eq. (5.20). At the end of the RG flow (i.e., for $\Lambda \to 1$ where $t_{\mathbf{k},\Lambda} \to t_{\mathbf{k}}$ and $\delta\mu_{\Lambda} \to \mu - \mu_0$) the two-point function is in this approximation given by

$$G_1(\mathbf{k},\omega) = \frac{Z_0}{i\omega - Z_0(t_{\mathbf{k}} - \delta\mu) + \mu_0},\tag{5.36}$$

with quasi-particle residue

$$Z_0 = 1 - \frac{n}{2}. (5.37)$$

Note that if we remove the counter-term $(\delta\mu=0)$, Eq. (5.36) can also be obtained from the Hubbard-I approximation (5.13) for the electronic single-particle Green function of the Hubbard model by taking the limit $U \to \infty$. At zero temperature where μ_0 vanishes the equation of state (5.35) then reduces to

$$n = \frac{2Z_0}{N} \sum_{\mathbf{k}} \Theta(\mu - t_{\mathbf{k}}). \tag{5.38}$$

In terms of the hole-doping x = 1 - n this can be written as

$$\frac{1-x}{1+x} = \frac{1}{N} \sum_{k} \Theta(\mu - t_{k}). \tag{5.39}$$

In Fig. \blacksquare we show the resulting filling n and hole-doping x as a function of the chemical potential μ for the t model with nearest neighbor hopping in a two-dimensional square lattice. Note that according to Eq. (5.34) the Fermi surface is for $T \to 0$ defined by

$$t_{\mathbf{k}_F} = \mu, \tag{5.40}$$

so that for $\mu=0$ where the Fermi surface covers half of the first Brillouin zone (see Fig. 2) we obtain x=1/3, corresponding to n=2/3. This clearly shows that Luttinger's theorem [32] (which states that in a Fermi liquid the volume of the Fermi surface is proportional to the electronic density) is violated in the t model [33]. The violation of Luttinger's theorem in the t model is a consequence of the projected Hilbert space.

The equation of state (5.38) has been obtained by approximating the self-energy $\Sigma_{\Lambda}(K)$ by its atomic limit given in Eq. (5.32). To go beyond this approximation, we now use the Wetterich equation (4.38) for the t-J model in the limit J=0 to derive a formally exact flow equation for the self-energy $\Sigma_{\Lambda}(K)$ of the t model. For

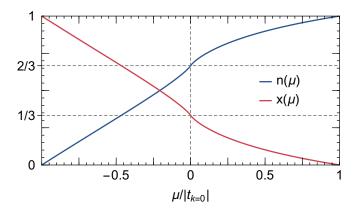


FIG. 1. Lattice filling n and corresponding hole doping x=1-n of the t model for nearest neighbor hopping on a square lattice as a function of the chemical potential μ . The graph has been obtained from the numerical solution of the approximate equation of state (5.39) with $t_k = -2t[\cos(k_x a) + \cos(k_y a)]$ where t > 0 and a is the lattice spacing.

vanishing J the flow in the fermionic sector decouples from the bosonic sector, so that the flow equation of the fermionic self-energy of the t model is formally identical to the flow equation of the self-energy of a system of canonical fermions $\boxed{3}$

$$\partial_{\Lambda} \Sigma_{\Lambda}(K) = \int_{K'} \sum_{\sigma'} \dot{G}_{\Lambda}(K')$$

$$\times \Gamma_{\Lambda}^{\bar{\psi}\bar{\psi}\psi\psi}(K\sigma, K'\sigma'; K'\sigma', K\sigma), \quad (5.41)$$

where the single-scale propagator is

$$\dot{G}_{\Lambda}(K) = G_{\Lambda}^{2}(K)\partial_{\Lambda} (t_{\mathbf{k},\Lambda} - \delta\mu_{\Lambda}). \tag{5.42}$$

The exact flow equation of the four-point vertex $\Gamma^{\psi\psi\psi\psi}_{\Lambda}(K\sigma, K'\sigma'; K'\sigma', K\sigma)$ involves the six-point vertex and can be found in Refs. 3 and 34. These vertices are related via skeleton equations to the corresponding connected correlation functions 3. In a simple level-1 truncation, we now approximate the flowing four-point vertex on the right-hand side of the flow equation (5.41) by its initial value for vanishing hopping. In principle the corresponding four-point correlation function can be obtained using the recursive algorithm for the Matsubara kernel functions recently derived by Halbinger et al. 35. A more direct method which we have previously used to calculate the initial vertices in our recently developed spin-FRG approach to dimerized spin systems [13] is presented in Appendix A and applied in Appendix C. For our purpose we need the four-point vertex only for the special combinations of spin labels $\sigma_1' = \sigma_2' = \sigma_2 = \sigma_1 = \sigma$ and $\sigma_1' = \sigma_1 = \sigma = -\sigma_2' = -\sigma_2$. When all spin projections

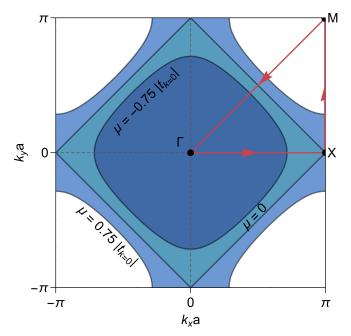


FIG. 2. Fermi surface of the t model with nearest-neighbor hopping on a square lattice for $\mu=0,\ 0.75\,|t_{k=0}|$ and $-0.75\,|t_{k=0}|$. Although the Fermi surface at $\mu=0$ covers half of the first Brillouin zone, the corresponding filling is n<1 due to the projected Hilbert space. The black dots denote the high symmetry points $\mathbf{\Gamma}=(0,0),\ \mathbf{X}=(\pi,0)$ and $\mathbf{M}=(\pi,\pi)$. The red arrows show the path through the Brillouin zone taken in Fig. 3

are equal we obtain

$$\Gamma_0^{\bar{\psi}\bar{\psi}\psi\psi}(\omega\sigma,\omega'\sigma;\omega'\sigma,\omega\sigma)$$

$$= -\frac{\beta}{Z_0^3} \frac{n_0}{2} (1 - \delta_{\omega,\omega'})(i\omega + \mu_0)(i\omega' + \mu_0), \qquad (5.43)$$

while for the interaction between two projected fermions with opposite spin we find

$$\Gamma_0^{\bar{\psi}\bar{\psi}\psi\psi}(\omega\sigma,\omega'\bar{\sigma};\omega'\bar{\sigma},\omega\sigma) = -\frac{i\omega + i\omega' + 2\mu_0}{Z_0^3} + \frac{\beta}{Z_0^4} \frac{n_0}{2} \left(\frac{n_0}{2} + \delta_{\omega,\omega'}\right) (i\omega + \mu_0)(i\omega' + \mu_0).$$
(5.44)

Here, $\bar{\sigma} = -\sigma$ denotes the inverted spin projection and we have omitted the momentum labels because in the atomic limit the vertices depended only on the frequency part ω of the collective labels $K = (\mathbf{k}, \omega)$. Note also that now $Z_0 = 1 - \frac{n_0}{2}$, since we no longer require the filling to remain constant during the flow. Substituting the initial values (5.43) and (5.44) for the four-point vertex into the flow equation (5.41), we obtain

$$\partial_{\Lambda} \Sigma_{\Lambda}(\omega) = \frac{(i\omega + \mu_0)^2}{Z_0^4} \frac{n_0}{2} \left(2 - \frac{n_0}{2} \right) A_{\Lambda}(\omega) - \frac{(i\omega + \mu_0)}{Z_0^3} \left[B_{\Lambda} + \frac{n_0}{2} \left(1 - n_0 \right) \frac{\beta}{Z_0} C_{\Lambda} \right] - \frac{C_{\Lambda}}{Z_0^3}, \quad (5.45)$$

where

such that

$$\partial_{\Lambda} \Sigma_{\Lambda}(0) = \frac{\mu_0^2}{Z_0^4} \frac{n_0}{2} \left(2 - \frac{n_0}{2} \right) A_{\Lambda}(0) - \frac{\mu_0}{Z_0^3} B_{\Lambda}$$
$$- \left[\frac{n_0 (1 - n_0)}{2Z_0^4} \tilde{\mu}_0 + \frac{1}{Z_0^3} \right] C_{\Lambda}$$
$$= 0, \tag{5.47}$$

$$A_{\Lambda}(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \dot{G}_{\Lambda}(\mathbf{k}, \omega), \qquad (5.46a)$$

$$B_{\Lambda} = \frac{1}{\beta N} \sum_{\mathbf{k}\omega'} \dot{G}_{\Lambda}(\mathbf{k}, \omega'), \tag{5.46b}$$

$$C_{\Lambda} = \frac{1}{\beta N} \sum_{\mathbf{k}\omega'} \dot{G}_{\Lambda}(\mathbf{k}, \omega') (i\omega' + \mu_0).$$
 (5.46c)

A comprehensive analysis of the flow equation (5.45) will be presented elsewhere [36]. Here, we focus for simplicity on the limit $T \to 0$ where $\mu_0 \to 0$. To satisfy the condition (5.33) we should then choose the counter-term μ_{Λ}

where $\tilde{\mu}_0 = \beta \mu_0$ is independent of temperature; see Eq. (5.20). Equation (5.47) can be satisfied by choosing the counter-term μ_{Λ} such that

$$C_{\Lambda} = \frac{\mu_0}{1 + \frac{n_0}{2} \frac{1 - n_0}{Z_0} \tilde{\mu}_0} \left[\frac{n_0}{2} \frac{\left(2 - \frac{n_0}{2}\right)}{Z_0} \mu_0 A_{\Lambda}(0) - B_{\Lambda} \right], \tag{5.48}$$

which together with the initial condition $\Sigma_0(0) = -\mu_0/Z_0 \to 0$ at $T \to 0$ guarantees that $\Sigma_{\Lambda}(0)$ vanishes at zero temperature for all values of the deformation parameter Λ . At T=0 the condition (5.48) reduces to $C_{\Lambda}=0$. Solving for $\partial_{\Lambda}\mu_{\Lambda}$, we conclude that at T=0 the scale-dependent chemical potential μ_{Λ} is determined by the flow equation

$$\partial_{\Lambda}\mu_{\Lambda} = \frac{\frac{1}{\beta N} \sum_{\mathbf{k}\omega'} (\partial_{\Lambda} t_{\mathbf{k},\Lambda}) G_{\Lambda}^{2}(\mathbf{k},\omega') i\omega'}{\frac{1}{\beta N} \sum_{\mathbf{k}\omega'} G_{\Lambda}^{2}(\mathbf{k},\omega') i\omega'}.$$
 (5.49)

Replacing C_{Λ} according to Eq. (5.48), the flow equation (5.45) for the self-energy becomes

$$\partial_{\Lambda} \Sigma_{\Lambda}(\omega) = -\frac{i\omega}{1 + \frac{n_0}{2} \frac{1 - n_0}{Z_0} \tilde{\mu}_0} \frac{B_{\Lambda}}{Z_0^3} + \frac{\frac{n_0}{2} (2 - \frac{n_0}{2})}{Z_0^4} \left[\frac{(i\omega + \mu_0)^2}{N} \sum_{\mathbf{k}} \frac{\partial_{\Lambda} (t_{\mathbf{k},\Lambda} - \mu_{\Lambda})}{[t_{\mathbf{k},\Lambda} - \mu_{\Lambda} + \Sigma_{\Lambda}(\omega)]^2} - \left(\mu_0 + \frac{i\omega}{1 + \frac{2}{n_0} \frac{Z_0}{(1 - n_0)\tilde{\mu}_0}} \right) \frac{\mu_0}{N} \sum_{\mathbf{k}} \frac{\partial_{\Lambda} (t_{\mathbf{k},\Lambda} - \mu_{\Lambda})}{[t_{\mathbf{k},\Lambda} - \mu_{\Lambda} + \Sigma_{\Lambda}(0)]^2} \right], \quad (5.50)$$

which should be integrated with the initial condition

$$\Sigma_{\Lambda=0}(\omega) = \Sigma_0(\omega) = -\frac{i\omega + \mu_0}{Z_0}, \qquad Z_0 = 1 - \frac{n_0}{2}.$$
 (5.51)

To make progress analytically, we next modify the flow equation (5.50) using the so-called Katanin substitution (37), which has been shown to reduce the errors due to the violation of Ward identities by truncations of the FRG flow equations for canonical fermions. For the flow equation (5.50), the Katanin substitution amounts to replacing the single-scale propagator $\dot{G}_{\Lambda}(K)$ by the total Λ -derivative of the scale-dependent propagator $G_{\Lambda}(K)$; i.e.,

$$\frac{\partial_{\Lambda}(t_{\mathbf{k},\Lambda} - \mu_{\Lambda})}{\left[t_{\mathbf{k},\Lambda} - \mu_{\Lambda} + \Sigma_{\Lambda}(\omega)\right]^{2}} \to \partial_{\Lambda} \left[\frac{-1}{t_{\mathbf{k},\Lambda} - \mu_{\Lambda} + \Sigma_{\Lambda}(\omega)}\right]. \tag{5.52}$$

Then both sides of the flow equation Eq. (5.50) become total Λ -derivatives, so that we may explicitly integrate it over the flow parameter Λ . With the Katanin substitution, the contribution from the first term in Eq. (5.50) involving B_{Λ} becomes proportional to the difference between initial and final fillings,

$$\int_0^1 d\Lambda B_{\Lambda} \to \frac{1}{\beta N} \sum_{\mathbf{k}\omega} \left[G(\mathbf{k}, \omega) + \frac{1}{\Sigma_0(\omega)} \right] = \frac{n}{2} - \frac{1}{\beta} \sum_{\omega} \frac{Z_0}{i\omega + \mu_0} e^{i\omega 0^+} = \frac{n - n_0}{2}. \tag{5.53}$$

Here, we have used Eqs. (5.19) and (5.20) to express the Matsubara sum in terms of the filling,

$$\frac{1}{\beta} \sum_{\omega} \frac{Z_0}{i\omega + \mu_0} e^{i\omega 0^+} = \frac{1 - \frac{n_0}{2}}{e^{-\beta\mu_0} + 1} = \frac{e^{\beta\mu_0}}{1 + 2e^{\beta\mu_0}} = \frac{n_0}{2}.$$
 (5.54)

With the initial condition (5.51), we thus find that the self-energy $\Sigma(\omega)$ satisfies for $T \to 0$ the following implicit equation:

$$\Sigma(\omega) = -\frac{i\omega}{Z_0} - \frac{i\omega}{Z_0^3} \frac{1}{1 + \frac{n_0}{2} \frac{1 - n_0}{Z_0} \tilde{\mu}_0} \frac{n - n_0}{2} + \frac{i\omega}{Z_0^3} \frac{n_0}{2} \left(2 - \frac{n_0}{2}\right) \left[\frac{1}{1 + \frac{2}{n_0} \frac{Z_0}{(1 - n_0)\tilde{\mu}_0}} - \frac{1}{N} \sum_{\mathbf{k}} \frac{t_{\mathbf{k}} - \mu + \Sigma(\omega) + \frac{i\omega}{Z_0}}{t_{\mathbf{k}} - \mu + \Sigma(\omega)}\right]. \quad (5.55)$$

For $\omega \to 0$ this yields to leading order

$$\Sigma(\omega) = -\frac{i\omega}{Z} + \mathcal{O}(\omega^2), \tag{5.56}$$

where

$$\frac{1}{Z} = \frac{1}{Z_0} + \frac{1}{Z_0^3} \frac{1}{1 + \frac{n_0}{2} \frac{1 - n_0}{Z_0} \tilde{\mu}_0} \left[\frac{n_0}{2} \left(2 - \frac{n_0}{2} \right) + \frac{n - n_0}{2} \right]
= \frac{1}{Z_0} + \frac{1}{Z_0^3} \frac{1}{1 + \frac{n_0}{2} \frac{1 - n_0}{Z} \tilde{\mu}_0} \left[\frac{n + n_0}{2} - \frac{n_0^2}{4} \right].$$
(5.57)

We conclude that the effective kinematic interaction due to the Hilbert space projection reduces the quasi-particle residue to

$$Z = Z_0^3 \frac{1 + \frac{x_0 n_0}{2 Z_0} \tilde{\mu}_0}{1 + \frac{x_0 n_0}{2} \tilde{\mu}_0 Z_0 + \frac{n - n_0}{2}},$$
 (5.58)

where we have again introduced the hole doping $x_0 = 1 - n_0$. To estimate the quasi-particle damping, we substitute the low-energy expansion (5.56) for the self-energy on the right-hand side of Eq. (5.55) and analytically continue both sides to real frequencies to obtain the retarded self-energy $\Sigma^R(\omega) = \Sigma(\omega)|_{i\omega\to\omega+i0^+}$. Taking the imaginary part yields

$$\operatorname{Im}\Sigma^{R}(\omega) = -\pi \frac{n_{0}}{2} \left(2 - \frac{n_{0}}{2} \right) \frac{Z}{Z_{0}^{4}} \frac{\omega^{2}}{N} \sum_{\mathbf{k}} \delta(\omega - Z[t_{\mathbf{k}} - \mu]).$$

$$(5.59)$$

In terms of the (bare) density of states

$$\nu_0(\epsilon) = \frac{1}{N} \sum_{\mathbf{k}} \delta(\epsilon - t_{\mathbf{k}})$$
 (5.60)

this can be written as

$$Z \text{Im} \Sigma^{R}(\omega) = -\pi \frac{n_0}{2} \left(2 - \frac{n_0}{2} \right) \frac{Z}{Z_0^4} \omega^2 \nu_0(\mu + \omega/Z).$$
(5.61)

We conclude that at low-energies the retarded propagator of the projected fermions in the t model has the quasi-particle form

$$G^{R}(\omega) = \frac{Z}{\omega - \xi_{\mathbf{k}} + i\gamma_{\mathbf{k}}},\tag{5.62}$$

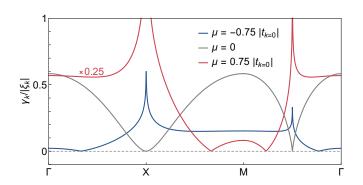


FIG. 3. Momentum dependence of the damping coefficient $\gamma_{k}/|\xi_{k}|$ on a square lattice, plotted along the path shown in Fig. $\boxed{2}$ for chemical potential $\mu=0,\ 0.75\,|t_{k=0}|$ and $-0.75\,|t_{k=0}|$. Note that the damping becomes arbitrarily small in the vicinity of the Fermi surface, indicating well-defined quasi-particles. The singularities in the damping for $\mu\neq 0$ reflect the van-Hove singularities of the two-dimensional density of states.

where the quasi-particle residue Z is given in Eq. (5.58), the quasi-particle dispersion is

$$\xi_{\mathbf{k}} = Z(t_{\mathbf{k}} - \mu) = Z(t_{\mathbf{k}} - t_{\mathbf{k}_F}), \tag{5.63}$$

and the quasi-particle damping is

$$\gamma_{\mathbf{k}} = -Z \operatorname{Im} \Sigma^{R} (\omega = \xi_{\mathbf{k}})$$

$$= \pi \frac{n_{0}}{2} \left(2 - \frac{n_{0}}{2} \right) \frac{Z}{Z_{0}^{4}} \nu_{0}(t_{\mathbf{k}}) \xi_{\mathbf{k}}^{2}. \tag{5.64}$$

Recall that according to Eq. (5.40), we have constructed our counter-term such that for vanishing temperature the Fermi surface is given by $t_{k_F} = \mu$. To explicitly calculate the chemical potential μ for a given lattice filling we should integrate the flow equation (5.49) for the counterterm. The results of this calculation will be reported elsewhere (36). As an estimate we may use the approximate equation of state (5.38) with $n \approx n_0$; see Fig. (3)

Our results [5.62] 5.64 imply that at zero temperature the t model supports well-defined quasi-particles in the sense that the quasi-particle residue is finite and the ratio $\gamma_{\mathbf{k}}/\xi_{\mathbf{k}}$ of the quasi-particle damping to the excitation energy becomes arbitrarily small for $\mathbf{k} \to \mathbf{k}_F$, provided that

the density of states is finite. Thus we find the ground state of the t model to be a hidden Fermi liquid 28 - 30, which in this respect behaves just like an ordinary Fermi liquid. However, due to the projected Hilbert space Luttinger's theorem is violated in a hidden Fermi liquid.

Let us conclude this section with a caveat. Within our level-1 truncation of the FRG flow equations the effective interaction does not have any momentum dependence, so that our self-energy depends only on frequency. While in reduced dimensions this approximation is probably not justified, we expect it to be valid in three and higher dimensions because in the limit of infinite dimensions (which can be realized by a proper rescaling of the hopping) the self-energy of the Hubbard model is known to be momentum-independent [38] [39]. Unfortunately, the limit of infinite on-site repulsion is not easily accessible within dynamical mean-field theory, so that we cannot compare the results obtained in this section with numerical calculations based on dynamical mean-field theory.

VI. SUMMARY AND OUTLOOK

In this work, we have developed a new functional renormalization group approach to strongly correlated electronic lattice models with projected Hilbert spaces using Hubbard X-operators. Our approach is complementary to the usual truncated vertex expansion for fermionic many-body systems 3+5, 40, which breaks down at intermediate coupling. The main advantage of our X-FRG approach is that the kinematic constraints imposed by the Hilbert space projection can be taken into account non-perturbatively. The X-FRG approach relies on the simple insight that formally exact FRG flow equations for generating functionals can be derived even if the Hamiltonian cannot be expressed in terms of operators satisfying canonical commutation relations. In previous works 7 14 we have shown that this insight can be used to derive exact flow equations for the time-ordered spin correlation functions of quantum spin systems. Although a diagrammatic representation of perturbation theory in terms of Hubbard X-operators has been developed 15-17, the diagrammatic structure is rather complicated. On the other hand, the diagrammatic representation of the flow equations for the irreducible vertices obtained within our X-FRG approach is identical to the familiar diagrammatics 3 generated by the usual Wetterich equation 6 for fermionic or bosonic many-body systems.

To demonstrate that the X-FRG can indeed be used to obtain useful results for strongly correlated electrons, in Sec. We have presented two simple applications. On the one hand, we have shown that the so-called Hubbard-I approximation can be obtained simply by approximating the irreducible two-point vertices by their initial conditions corresponding to the atomic limit. More importantly, we have used our X-FRG approach to calculate the single-particle Green function in the hidden Fermi

liquid state 28-30 of the Hubbard model at infinite on-site repulsion (i.e., the t model). In this case Luttinger's theorem 32, stating that in a normal Fermi liquid the volume of the Fermi surface is proportional to the density, is violated due to the projected Hilbert space. Nevertheless, the quasi-particles for momenta in the vicinity of the Fermi surface are well-defined in the sense that their damping is small compared with their excitation energy. Our calculation of the quasi-particle damping of the t model presented in Sec. V is rather simple and elegant; we are not aware of any other analytical method which is able to calculate the quasi-particle damping in strongly correlated systems with projected Hilbert spaces. Although the quasi-particle energies can also be estimated by means a Gutzwiller projection 41-43 of a suitable variational state, to the best of our knowledge the quasi-particle damping has so far not been obtained from Gutzwiller projections.

Our X-FRG approach can be extended in many directions which we are planning to explore in future publications. Possible applications include the interplay between fermionic quasi-particle excitations and spin- and charge fluctuations in the t-J model 44 45, the development of systematic strong-coupling expansions in powers of the hopping, or the study of the dynamics of holes in an antiferromagnetic background 46 48. It would also be interesting to explore the connection between our X-FRG approach and the dual fermion approach 49, which also relies on the local strong-coupling limit as a non-perturbative starting point.

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APPENDIX A: GENERALIZED SPECTRAL REPRESENTATION

In the X-FRG approach, the initial conditions of the flow equations generally involve the exact correlation functions of a solvable quantum-mechanical system. In this appendix, we therefore give a scheme to efficiently construct imaginary-time ordered correlation functions for any diagonalizable Hamiltonian \mathcal{H} with operators in an explicit matrix representation. Note that a related algorithm for this purpose has recently been discussed by Halbinger $et\ al.\ 35$. Our aim is to evaluate the imaginary-time ordered correlation function in Matsubara frequency space given by

$$\beta \delta_{\omega_1 + \dots + \omega_n, 0} C^{\alpha_1 \dots \alpha_n}(\omega_1, \dots, \omega_n) = \int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_n e^{i(\omega_1 \tau_1 + \dots + \omega_n \tau_n)} \left\langle \mathcal{T} \left\{ A^{\alpha_1}(\tau_1) \dots A^{\alpha_n}(\tau_n) \right\} \right\rangle. \tag{A1}$$

Here, $A^{\alpha}(\tau)$ denotes an arbitrary operator with flavor index α and imaginary-time dependence given by

$$A^{\alpha}(\tau) = e^{\mathcal{H}\tau} A^{\alpha} e^{-\mathcal{H}\tau}.$$
 (A2)

The imaginary-time ordering operator \mathcal{T} acts as

$$\mathcal{T}\left\{A^{\alpha_{1}}(\tau_{1})A^{\alpha_{2}}(\tau_{2})\right\} = \Theta(\tau_{1} - \tau_{2})A^{\alpha_{1}}(\tau_{1})A^{\alpha_{2}}(\tau_{2}) + \zeta\Theta(\tau_{2} - \tau_{1})A^{\alpha_{2}}(\tau_{2})A^{\alpha_{1}}(\tau_{1}), \tag{A3}$$

where $\zeta = -1$ if both operators are of the Fermi type based on the classification introduced in Sec. III A otherwise $\zeta = 1$. The symbol

$$\langle \ldots \rangle = \frac{\operatorname{tr}[e^{-\beta \mathcal{H}} \ldots]}{\operatorname{tr}e^{-\beta \mathcal{H}}}$$
 (A4)

denotes the thermal expectation value. In order to evaluate it, we introduce the complete basis $|m_1\rangle,\ldots,|m_d\rangle$ of energy eigenstates with

$$\mathcal{H}\left|m_{j}\right\rangle = \epsilon_{m_{j}}\left|m_{j}\right\rangle. \tag{A5}$$

Here, the ϵ_{m_j} are the corresponding eigenenergies. We also introduce the partition function $\mathcal{Z} = \operatorname{tr} e^{-\beta \mathcal{H}} = \sum_m e^{-\beta \epsilon_m}$ and $\epsilon_{ij} = \epsilon_{m_i} - \epsilon_{m_j}$. Performing the time-ordering and relabeling the integration variables appropriately allows us to separate the right-hand side of Eq. (A1) into a universal frequency dependent coefficient $\Omega^{(n)}$ and a matrix product of operators:

$$\int_{0}^{\beta} d\tau_{1} \int_{0}^{\tau_{1}} d\tau_{2} \dots \int_{0}^{\tau_{n-1}} d\tau_{n} \sum_{\mathcal{P}} \sum_{\{m_{i}\}} \left[\zeta^{\mathcal{P}} \left(\frac{e^{-\beta \epsilon_{m_{1}}}}{\mathcal{Z}} \prod_{i=1}^{n} e^{(i\omega_{P(i)} + \epsilon_{i(i+1)})\tau_{i}} \right) \left(\prod_{i=1}^{n} \langle m_{i} | A^{\alpha_{P(i)}} | m_{i+1} \rangle \right) \right] \\
= \sum_{\mathcal{P}} \sum_{\{m_{i}\}} \zeta^{\mathcal{P}} \frac{e^{-\beta \epsilon_{m_{1}}}}{\mathcal{Z}} \Omega^{(n)} (\omega_{P(1)}, \dots, \omega_{P(n)}; \epsilon_{m_{1}}, \dots, \epsilon_{m_{n}}) \prod_{i=1}^{n} \langle m_{i} | A^{\alpha_{P(i)}} | m_{i+1} \rangle. \tag{A6}$$

Here, $\sum_{\{m_i\}}$ sums the eigenenergies and operator projections over all eigenstates. The $\sum_{\mathcal{P}}$ represents a summation over all permutations of the tuple (ω_i, α_i) consisting of frequency and associated operator label that result from the time-ordering. The factor $\zeta^{\mathcal{P}}$ gives a minus sign whenever an uneven number of Fermi type operators has been commuted. The products are defined periodic such that $n+1\equiv 1$, which is a consequence of the cyclic invariance of the trace.

We now give a blueprint to construct the frequency dependent coefficients $\Omega^{(n)}$ to any given order n. The integration procedure is in itself quite straightforward. However due to the Matsubara character of the frequencies that fulfill

$$e^{i\omega_i\beta} = \zeta = \pm 1,$$
 (A7)

the expression becomes ill defined with respect to various limits. Those limits should be taken into account while still treating the frequencies as continuous, giving rise to terms with additional constraints on the Matsubara frequency conservation. These terms correspond to the anomalous contributions presented by Halbinger *et al.* 35. To systematically identify all possible divergen-

cies and properly account for them, we modify the evaluation. For example, the innermost integral shall give either

$$\int_0^{\tau_{n-1}} d\tau_n e^{(i\omega_n + \epsilon_{n1})\tau_n} = \begin{cases} \delta_{\omega_n, 0} \delta_{\epsilon_{n1}, 0} \tau_{n-1} & \text{or} \\ \frac{e^{(i\omega_n + \epsilon_{n1})\tau_{n-1}} - 1}{i\omega_n + \epsilon_{n1}} \end{cases}$$
(A8)

This distinction is made within each integration, even though the limit of vanishing frequency and energy difference is for the moment well-defined in the second case of Eq. (A8). The complete result to any order is given by the sum of all possible branches emerging from taking all possible combinations of these different cases. The relation (A7) can then be applied without the need to consider any more limits. Additionally, due to energy conservation only terms proportional to $\delta_{\omega_1+\ldots+\omega_n,0}$ will appear in the final expression and each frequency Kronecker delta will be accompanied by a factor of β .

A general formula for this construction procedure is given by

$$\Omega^{(n)}(\omega_{1}, \dots, \omega_{n}; \epsilon_{m_{1}}, \dots, \epsilon_{m_{n}}) = \sum_{l=1}^{n} \frac{\beta^{l}}{l!} \sum_{b_{1}=1}^{n-1} \sum_{b_{2}>b_{1}}^{n-1} \dots \sum_{b_{l-1}>b_{l-2}}^{n-1} g_{1,b_{1}}(\omega_{1}, \dots, \omega_{b_{1}}; \epsilon_{m_{1}}, \dots, \epsilon_{m_{b_{l}+1}})
\times g_{b_{1}+1,b_{2}}(\omega_{b_{1}+1}, \dots, \omega_{b_{2}}; \epsilon_{m_{b_{1}+1}}, \dots, \epsilon_{m_{b_{2}+1}}) \dots g_{b_{l-1}+1,n}(\omega_{b_{l-1}+1}, \dots, \omega_{n}; \epsilon_{m_{b_{l-1}+1}}, \dots, \epsilon_{m_{n}}, \epsilon_{m_{1}}).$$
(A9)

$$\frac{\beta^{1}}{1!} \left\{ (\omega_{1} \quad \omega_{2} \quad \omega_{3} \quad \omega_{4}) \quad \propto \delta_{\omega_{1} + \omega_{2} + \omega_{3} + \omega_{4}, 0} \right.$$

$$\frac{\beta^{2}}{2!} \left\{ (\omega_{1} \quad \omega_{2} \quad \omega_{3} \quad \omega_{4}) \quad \propto \delta_{\omega_{1}, 0} \delta_{\omega_{2} + \omega_{3} + \omega_{4}, 0} \right.$$

$$\left. (\omega_{1} \quad \omega_{2} \quad \omega_{3} \quad \omega_{4}) \quad \propto \delta_{\omega_{1} + \omega_{2}, 0} \delta_{\omega_{3} + \omega_{4}, 0} \right.$$

$$\left. (\omega_{1} \quad \omega_{2} \quad \omega_{3} \mid_{b_{1}} \omega_{4}) \quad \propto \delta_{\omega_{1} + \omega_{2} + \omega, 03} \delta_{\omega_{4}, 0} \right.$$

$$\frac{\beta^{3}}{3!} \left\{ (\omega_{1} \mid_{b_{1}} \omega_{2} \quad \omega_{3} \mid_{b_{2}} \omega_{4}) \quad \propto \delta_{\omega_{1}, 0} \delta_{\omega_{2}, 0} \delta_{\omega_{3} + \omega_{4}, 0} \right.$$

$$\left. (\omega_{1} \quad \omega_{2} \mid_{b_{1}} \omega_{3} \mid_{b_{2}} \omega_{4}) \quad \propto \delta_{\omega_{1}, 0} \delta_{\omega_{2} + \omega_{3}, 0} \delta_{\omega_{4}, 0} \right.$$

$$\left. \frac{\beta^{4}}{4!} \left\{ (\omega_{1} \mid_{b_{1}} \omega_{2} \mid_{b_{2}} \omega_{3} \mid_{b_{3}} \omega_{4}) \quad \propto \delta_{\omega_{1}, 0} \delta_{\omega_{2}, 0} \delta_{\omega_{3}, 0} \delta_{\omega_{4}, 0} \right. \right.$$

FIG. 4. Construction scheme of all relevant summands of one permutation for the frequency dependent coefficient $\Omega^{(4)}$ of the four-point correlation function. The colored bars represent the summation indices of Eq. (A9) that count the allowed partitions.

Here, the nested sums over the variables b_i construct all possible stars and bars partitions 50 using l-1 bars of an ordered list given by the frequency arguments. An illustrative example for four frequencies is shown in Fig. 4 The contribution of a single partition is generated via the propagator function

$$g_{x,y}(\omega_x, \dots, \omega_y; \epsilon_x, \dots \epsilon_{y+1}) = \delta_{\sum_{j=x}^y \epsilon_{j(j+1)}, 0} \delta_{\sum_{j=x}^y \omega_j, 0} \prod_{j=1}^{y-x} \frac{1}{\sum_{i=1}^j \left[i\omega_{y-i+1} + \epsilon_{(y-i+1)(y-i+2)} \right]}.$$
(A10)

This term can be understood by following the nested imaginary-time integrations using the scheme shown in Eq. (A8), with the aim to create a specific frequency Kronecker delta containing j neighboring frequencies. The propagator product in Eq. (A10) is then a consequence of the j-1 integrations necessary to obtain an exponential containing the desired sum of frequencies.

To give an explicit example, we construct the coefficient $\Omega^{(4)}$, which determines the four-point correlation function. We first consider the order $\{\omega_1, \omega_2, \omega_3, \omega_4\}$ and note that the frequencies should afterwards be permuted in accordance with Eq. (A9). Sorted by powers of β the coefficients have the structure

$$\Omega^{(4)}(\omega_1, \omega_2, \omega_3, \omega_4; \epsilon_{m_1}, \epsilon_{m_2}, \epsilon_{m_3}, \epsilon_{m_4}) = \frac{\beta^4}{4!} \Omega_4^{(4)} + \frac{\beta^3}{3!} \Omega_3^{(4)} + \frac{\beta^2}{2!} \Omega_2^{(4)} + \beta \Omega_1^{(4)}.$$
(A11)

The term proportional to β has only one possible parti-

tion accompanied by a non-trivial frequency dependence:

$$\Omega_{1}^{(4)} = \frac{\delta_{\omega_{1} + \omega_{2} + \omega_{3} + \omega_{4}, 0}}{i\omega_{4} + i\omega_{3} + i\omega_{2} + \epsilon_{21}} \times \frac{1}{i\omega_{4} + i\omega_{3} + \epsilon_{31}} \frac{1}{i\omega_{4} + \epsilon_{41}}.$$
(A12)

The higher-order coefficients are given by

$$\begin{split} \Omega_{2}^{(4)} &= \delta_{\omega_{1},0} \delta_{\epsilon_{12},0} \frac{\delta_{\omega_{2} + \omega_{3} + \omega_{4},0} \delta_{\epsilon_{21},0}}{i\omega_{4} + i\omega_{3} + \epsilon_{31}} \frac{1}{i\omega_{4} + \epsilon_{41}} \\ &+ \frac{\delta_{\omega_{1} + \omega_{2},0} \delta_{\epsilon_{13},0}}{i\omega_{2} + \epsilon_{23}} \frac{\delta_{\omega_{3} + \omega_{4},0} \delta_{\epsilon_{31},0}}{i\omega_{4} + \epsilon_{41}} \\ &+ \frac{\delta_{\omega_{1} + \omega_{2} + \omega_{3},0} \delta_{\epsilon_{14},0}}{i\omega_{3} + i\omega_{2} + \epsilon_{24}} \frac{1}{i\omega_{3} + \epsilon_{34}} \delta_{\omega_{4},0} \delta_{\epsilon_{41},0}, \quad (A13) \end{split}$$

and

$$\Omega_{3}^{(4)} = \delta_{\omega_{1},0}\delta_{\epsilon_{12},0}\delta_{\omega_{2},0}\delta_{\epsilon_{23},0}\frac{\delta_{\omega_{3}+\omega_{4},0}\delta_{\epsilon_{31},0}}{i\omega_{4} + \epsilon_{41}}
+ \delta_{\omega_{1},0}\delta_{\epsilon_{12},0}\frac{\delta_{\omega_{2}+\omega_{3},0}\delta_{\epsilon_{24},0}}{i\omega_{3} + \epsilon_{34}}\delta_{\omega_{4},0}\delta_{\epsilon_{41},0}
+ \frac{\delta_{\omega_{1}+\omega_{2},0}\delta_{\epsilon_{13},0}}{i\omega_{2} + \epsilon_{23}}\delta_{\omega_{3},0}\delta_{\epsilon_{34},0}\delta_{\omega_{4},0}\delta_{\epsilon_{41},0}.$$
(A14)

Finally, the highest order of β will then include 4-1 bars, dividing this list in four single frequencies:

$$\Omega_4^{(4)} = \delta_{\omega_1,0} \delta_{\epsilon_{12},0} \delta_{\omega_2,0} \delta_{\epsilon_{23},0} \delta_{\omega_3,0} \delta_{\epsilon_{34},0} \delta_{\omega_4,0} \delta_{\epsilon_{41},0}. \quad (A15)$$

The structure of these terms is independent of the physical model, so that it is sufficient to construct them once. The general recipe for order n coefficients can be summarized as follows:

- Begin by considering a single permutation given by the tuple list $\{(\omega_1, \alpha_1), \dots, (\omega_n, \alpha_n)\}.$
- For each order $\beta^k/k!$ with $k \in [1, n]$, find all possible Kronecker delta combinations. This is equivalent to finding all possible stars and bars partitions of the ordered tuple list with k-1 bars.
- Multiply each Kronecker delta with suitable frequency dependent propagator functions (A10) according to Eq. (A9).

APPENDIX B: TWO-POINT FUNCTIONS OF X-OPERATORS IN THE HUBBARD ATOM

In this appendix, we calculate the two-point correlation functions of the X-operators of the Hubbard atom; i.e., the Hubbard model for vanishing hopping with Hamiltonian

$$\mathcal{H}_1 = \sum_{i} \left[U n_{i\uparrow} n_{i\downarrow} - \mu n_i - h S_i^z \right] = \sum_{ia} \epsilon_a X_i^{aa}, \quad (B1)$$

where for fixed chemical potential μ and magnetic field h the energies ϵ_a are

$$\epsilon_0 = 0, \quad \epsilon_{\uparrow} = -\mu - \frac{h}{2}, \quad \epsilon_{\downarrow} = -\mu + \frac{h}{2}, \quad \epsilon_2 = U - 2\mu.$$
(B2)

The generating functional of imaginary-time ordered connected correlation functions of the X-operators can then be written as

$$e^{\mathcal{G}_0[J]} = \operatorname{Tr}\left[e^{-\beta \mathcal{H}_1} \mathcal{T} e^{\int_0^\beta d\tau \sum_{i,p} J_i^p(\tau) X_i^p(\tau)}\right].$$
 (B3)

Since all sites are decoupled in this limit, the generating functional decouples into a sum of single-site generating functionals:

$$\mathcal{G}_0[J] = \sum_i \mathcal{G}_{\text{site}}[J_i],$$
 (B4)

where the generating functional of the single-site (atomic) correlation functions is

$$\mathcal{G}_{\text{site}}[J] = \ln \operatorname{tr} \left[e^{-\beta \mathcal{H}_{\text{site}}} \mathcal{T} e^{\int_0^\beta d\tau \sum_p J^p(\tau) X^p(\tau)} \right], \tag{B5}$$

with single-site Hamiltonian

$$\mathcal{H}_{\text{site}} = U n_{\uparrow} n_{\downarrow} - \mu n - h S^z = \sum_{a} \epsilon_a X^{aa}.$$
 (B6)

The symbol $\operatorname{tr}[\ldots]$ denotes the trace over the four-state fermionic Fock space associated with a single lattice site. The single-site functional $\mathcal{G}_{\operatorname{site}}[J]$ cannot be calculated in closed form, but can be expanded in powers of the sources,

$$\mathcal{G}_{\text{site}}[J] = \mathcal{G}_{\text{site}}[0] + \int_{0}^{\beta} d\tau \sum_{p} \langle X^{p}(\tau) \rangle J^{p}(\tau)
+ \frac{1}{2!} \int_{0}^{\beta} d\tau_{1} d\tau_{2} \sum_{p_{1}p_{2}} G_{0}^{p_{1}p_{2}}(\tau_{1}, \tau_{2}) J^{p_{1}}(\tau_{1}) J^{p_{2}}(\tau_{2})
+ \dots,$$
(B7)

where

$$G_0^{p_1 p_2}(\tau_1, \tau_2) = \langle \mathcal{T} \{ X^{p_2}(\tau_2) X^{p_1}(\tau_1) \} \rangle - \langle X^{p_2}(\tau_2) \rangle \langle X^{p_1}(\tau_1) \rangle.$$
 (B8)

Here, the thermal expectation value is evaluated with respect to the single-site Hamiltonian $\mathcal{H}_{\text{site}}$. The expectation values $\langle X^p(\tau) \rangle$ are only finite for the diagonal Bose type X-operators $p = 00, \uparrow \uparrow, \downarrow \downarrow, 22$. If we introduce only fermionic sources, the linear term is absent.

Let us now explicitly calculate the connected correlation functions of the Fermi type X-operators up to fourth order. Therefore we work with the occupation number basis of the four-dimensional single-site Fock space consisting of the vacuum state $|0\rangle$, the two single-particle states $|\uparrow\rangle = c^{\dagger}_{\uparrow}|0\rangle$ and $|\downarrow\rangle = c^{\dagger}_{\downarrow}|0\rangle$, and the antisymmetrized two-particle states $|2\rangle = c^{\dagger}_{\downarrow}c^{\dagger}_{\uparrow}|0\rangle = -c^{\dagger}_{\uparrow}c^{\dagger}_{\downarrow}|0\rangle$. Representing these states by

$$|0\rangle \to e_0 = \begin{pmatrix} 1\\0\\0\\0 \end{pmatrix}, \qquad |\uparrow\rangle \to e_{\uparrow} = \begin{pmatrix} 0\\1\\0\\0 \end{pmatrix},$$
$$|\downarrow\rangle \to e_{\downarrow} = \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix}, \qquad |2\rangle \to e_2 = \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix}, \qquad (B9)$$

the X-operators are represented by the matrices

$$X^{ab} \to \hat{X}^{ab} = \boldsymbol{e}_a \boldsymbol{e}_b^T, \quad a, b \in \{0, \uparrow, \downarrow, 2\},$$
 (B10)

and from Eq. (3.4) we conclude that the canonical creation and annihilation operators are represented by the

following 4×4 matrices,

$$\hat{c}_{\uparrow} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \hat{c}_{\uparrow}^{\dagger} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \quad (B11)$$

$$\hat{c}_{\downarrow} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \hat{c}_{\downarrow}^{\dagger} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad (B12)$$

where the lines emphasize the block-diagonal structure of the matrices. One easily verifies that these matrices satisfy the canonical anticommutation relations

$$\hat{c}_{\sigma}\hat{c}_{\sigma'}^{\dagger} + \hat{c}_{\sigma'}^{\dagger}\hat{c}_{\sigma} = \delta_{\sigma\sigma'}\hat{1}$$
 (B13)

and

$$\hat{c}_{\sigma}\hat{c}_{\sigma'} + \hat{c}_{\sigma'}\hat{c}_{\sigma} = \hat{0} = \hat{c}_{\sigma}^{\dagger}\hat{c}_{\sigma'}^{\dagger} + \hat{c}_{\sigma'}^{\dagger}\hat{c}_{\sigma}^{\dagger}. \tag{B14}$$

Here, $\hat{1}$ is the 4×4 unit matrix and $\hat{0}$ is the 4×4 null matrix. The occupation number operators are represented by

$$\hat{n}_{\uparrow} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \hat{n}_{\downarrow} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad (B15)$$

and the single-site Hamiltonian $\mathcal{H}_{\text{site}}$ in Eq. (B6) is represented by the diagonal matrix

$$\hat{H} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -\mu - \frac{h}{2} & 0 & 0 \\ 0 & 0 & -\mu + \frac{h}{2} & 0 \\ 0 & 0 & 0 & U - 2\mu \end{pmatrix} = \sum_{a} \epsilon_{a} \hat{X}^{aa}.$$
(B1)

Let us now calculate the two-point correlation functions of the X-operators,

$$\left\langle \mathcal{T} \left\{ \hat{X}^{a_1b_1}(\tau_1) \hat{X}^{a_2b_2}(\tau_2) \right\} \right\rangle - \left\langle \hat{X}^{a_1b_1}(\tau_1) \right\rangle \left\langle \hat{X}^{a_2b_2}(\tau_2) \right\rangle$$

$$= \frac{1}{\mathcal{Z}} \operatorname{tr} \left[e^{-\beta \hat{H}} \mathcal{T} \left\{ \hat{X}^{a_1b_1}(\tau_1) \hat{X}^{a_2b_2}(\tau_2) \right\} \right]$$

$$- \frac{1}{\mathcal{Z}^2} \operatorname{tr} \left[e^{-\beta \hat{H}} \hat{X}^{a_1b_1}(\tau_1) \right] \operatorname{tr} \left[e^{-\beta \hat{H}} \hat{X}^{a_2b_2}(\tau_2) \right], \tag{B17}$$

where the single-site partition function is explicitly

$$Z = \text{tr}e^{-\beta \hat{H}} = \sum_{a} e^{-\beta \epsilon_{a}}$$

$$= 1 + e^{\beta(\mu + \frac{h}{2})} + e^{\beta(\mu - \frac{h}{2})} + e^{\beta(2\mu - U)}, \quad (B18)$$

and

$$\hat{X}^{ab}(\tau) = e^{\hat{H}\tau} \hat{X}^{ab} e^{-\hat{H}\tau} = e^{(\epsilon_a - \epsilon_b)\tau} \hat{X}^{ab} = e^{-\epsilon_{ab}\tau} \hat{X}^{ab}.$$
(B19)

Here, the energy difference ϵ_{ab} is defined by

$$\epsilon_{ab} = \epsilon_b - \epsilon_a,$$
 (B20)

where the inverted order of labels on the right-hand side is introduced to emphasize the analogy with canonical fermions [51] and to facilitate the comparison with the notation introduced in the textbook [16]. Note that only the diagonal X-operators have a finite expectation value,

$$\bar{X}^{ab} = \langle \hat{X}^{ab} \rangle = \delta_{ab} x_a, \qquad x_a = \frac{e^{-\beta \epsilon_a}}{\mathcal{Z}},$$
 (B21)

where the x_a are the normalized ($\sum_a x_a = 1$) occupation probabilities of the states $|a\rangle$ in the atomic limit. The time-ordered connected two-point function for any pair of Fermi type X-operators is

$$\left\langle \mathcal{T} \left\{ \hat{X}^{a_1b_1}(\tau_1) \hat{X}^{a_2b_2}(\tau_2) \right\} \right\rangle
= -G_{a_1b_1}(\tau_1 - \tau_2) \left\langle [X^{a_1b_1}(\tau_2), X^{a_2b_2}(\tau_2)]_+ \right\rangle
= -G_{a_1b_1}(\tau_1 - \tau_2) \left(\delta_{b_1a_2} \left\langle X^{a_1b_2}(\tau_2) \right\rangle + \delta_{a_1b_2} \left\langle X^{a_2b_1}(\tau_2) \right\rangle \right)
= -G_{a_1b_1}(\tau_1 - \tau_2) \left(\delta_{b_1a_2} \bar{X}^{a_1b_2} + \delta_{a_1b_2} \bar{X}^{a_2b_1} \right)
= -G_{a_1b_1}(\tau_1 - \tau_2) \delta_{a_1b_2} \delta_{b_1a_2}(x_{a_2} + x_{b_2}).$$
(B22)

Here, $[\ ,\]_+$ denotes the anti-commutator and $G_{ab}(\tau)$ is formally identical to the imaginary-time propagator of non-interacting fermions at energy $\epsilon_{ab}=\epsilon_b-\epsilon_a$,

$$G_{ab}(\tau) = -e^{-\epsilon_{ab}\tau} [\Theta(\tau)(1 - n_{ab}) - \Theta(-\tau)n_{ab}], \quad (B23)$$

with the Fermi function

$$n_{ab} = \frac{1}{e^{\beta \epsilon_{ab}} + 1}. (B24)$$

On the other hand, for two non-diagonal Bose type X-operators we have

$$\left\langle \mathcal{T} \left\{ \hat{X}^{a_1b_1}(\tau_1) \hat{X}^{a_2b_2}(\tau_2) \right\} \right\rangle
= -G_{a_1b_1}(\tau_1 - \tau_2) \left\langle \left[X^{a_1b_1}(\tau_2), X^{a_2b_2}(\tau_2) \right] \right\rangle
= -G_{a_1b_1}(\tau_1 - \tau_2) \left(\delta_{b_1a_2} \left\langle X^{a_1b_2}(\tau_1) \right\rangle - \delta_{a_1b_2} \left\langle X^{a_2b_1}(\tau_1) \right\rangle \right)
= -G_{a_1b_1}(\tau_1 - \tau_2) \left(\delta_{b_1a_2} \bar{X}^{a_1b_2} - \delta_{a_1b_2} \bar{X}^{a_2b_1} \right)
= G_{a_1b_1}(\tau_1 - \tau_2) \delta_{a_1b_2} \delta_{b_1a_2}(x_{a_2} - x_{b_2}),$$
(B25)

where $G_{ab}(\tau)$ is now the usual imaginary-time propagator of non-interacting bosons,

$$G_{ab}(\tau) = -e^{-\epsilon_{ab}\tau} [\Theta(\tau)(1 + n_{ab}) + \Theta(-\tau)n_{ab}], \quad (B26)$$

where n_{ab} is now the Bose function,

$$n_{ab} = \frac{1}{e^{\beta \epsilon_{ab}} - 1}. (B27)$$

Both cases can be compactly written as

$$\left\langle \mathcal{T} \left\{ \hat{X}^{a_1 b_1}(\tau_1) \hat{X}^{a_2 b_2}(\tau_2) \right\} \right\rangle$$

$$= \zeta G_{a_1 b_1}^{\zeta}(\tau_1 - \tau_2) \delta_{a_1 b_2} \delta_{b_1 a_2}(x_{a_2} - \zeta x_{b_2})$$

$$= G_{a_1 b_1}^{\zeta}(\tau_1 - \tau_2) \delta_{a_1 b_2} \delta_{b_1 a_2}(\zeta x_{a_2} - x_{b_2}), \tag{B28}$$

where

$$G_{ab}^{\zeta}(\tau) = -e^{-\epsilon_{ab}\tau} [\Theta(\tau)(1+\zeta n_{ab}^{\zeta}) + \zeta \Theta(-\tau) n_{ab}^{\zeta}],$$
(B29)

and

$$n_{ab}^{\zeta} = \frac{1}{e^{\beta \epsilon_{ab}} - \zeta},\tag{B30}$$

with $\zeta=1$ for Bose type X-operators and $\zeta=-1$ for Fermi type X-operators. The functions $G^{\zeta}_{ab}(\tau-\tau')$ satisfy the usual Kubo-Martin-Schwinger boundary conditions, i.e., $G^{\zeta}_{ab}(\tau-\tau')$ is for $\zeta=-1$ anti-periodic in both times τ and τ' with period β , while for $\zeta=1$ it is periodic in both times. As a consequence, $G^{\zeta}_{ab}(\tau-\tau')$ can be represented as a Matsubara sum,

$$G_{ab}^{\zeta}(\tau) = \frac{1}{\beta} \sum_{\omega} e^{-i\omega\tau} G_{ab}(\omega), \qquad (B31)$$

where $\omega = 2\pi nT$ for $\zeta = 1$ and $\omega = 2\pi (n + \frac{1}{2})T$ for $\zeta = -1$. The Fourier coefficients depend on ζ only via the Matsubara frequencies,

$$G_{ab}(\omega) = \int_0^\beta d\tau e^{i\omega\tau} G_{ab}^{\zeta}(\tau) = \frac{1}{i\omega - \epsilon_{ab}}.$$
 (B32)

Actually, the simplest way to derive the two-point correlation function of the X-operators in frequency space is by direct calculation of the Fourier coefficients using $X^{ab}(\tau) = e^{-\epsilon_{ab}\tau}X^{ab}(0)$ and Eq. (A1) and (A6). The correlation function of two non-diagonal X-operators is

$$\int_0^\beta d\tau e^{i\omega\tau} \left\langle X^{a_1b_1}(\tau) X^{a_2b_2}(0) \right\rangle$$

$$= \delta_{a_1b_2} \delta_{b_1a_2} \frac{\zeta x_{a_2} - x_{b_2}}{i\omega - \epsilon_{a_1b_1}}.$$
(B33)

Note that according to the definition (B8) the two-point function of non-diagonal X-operators has the inverted ordering of the labels,

$$G_0^{a_1b_1, a_2b_2}(\tau_1, \tau_2) = \left\langle \mathcal{T} \left\{ \hat{X}^{a_2b_2}(\tau_2) \hat{X}^{a_1b_1}(\tau_1) \right\} \right\rangle$$
$$= G_{a_2b_2}^{\zeta}(\tau_2 - \tau_1) \delta_{a_1b_2} \delta_{b_1a_2}(\zeta x_{a_1} - x_{b_1}). \tag{B34}$$

In frequency space this becomes

$$\begin{split} \tilde{G}_{0}^{a_{1}b_{1},a_{2}b_{2}}(\omega_{1},\omega_{2}) \\ &= \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} e^{i(\omega_{1}\tau_{1}+\omega_{2}\tau_{2})} G_{0}^{a_{1}b_{1},a_{2}b_{2}}(\tau_{1},\tau_{2}) \\ &= \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} e^{i(\omega_{1}\tau_{1}+\omega_{2}\tau_{2})} G_{a_{2}b_{2}}(\tau_{2}-\tau_{1}) \\ &\qquad \qquad \times \delta_{a_{1}b_{2}} \delta_{b_{1}a_{2}}(\zeta x_{a_{1}}-x_{b_{1}}) \\ &= \beta \delta_{\omega_{1}+\omega_{2},0} \delta_{a_{1}b_{2}} \delta_{b_{1}a_{2}} \frac{\zeta x_{a_{1}}-x_{b_{1}}}{i\omega_{2}-\epsilon_{a_{2}b_{2}}} \\ &= \beta \delta_{\omega_{1}+\omega_{2},0} \delta_{a_{1}b_{2}} \delta_{b_{1}a_{2}} \frac{x_{b_{1}}-\zeta x_{a_{1}}}{i\omega_{1}-\epsilon_{a_{1}b_{1}}} \\ &= \beta \delta_{\omega_{1}+\omega_{2},0} \delta_{a_{1}b_{2}} \delta_{b_{1}a_{2}} \left[\frac{x_{b_{1}}}{i\omega_{1}-\epsilon_{a_{1}b_{1}}} + \zeta \frac{x_{b_{2}}}{i\omega_{2}-\epsilon_{a_{2}b_{2}}} \right], \end{split}$$
(B35)

which is manifestly (anti)-symmetric with respect to the exchange $1 \leftrightarrow 2$; i.e.,

$$\tilde{G}_0^{a_1b_1, a_2b_2}(\omega_1, \omega_2) = \zeta \tilde{G}_0^{a_2b_2, a_1b_1}(\omega_2, \omega_1).$$
 (B36)

For completeness let us also give the propagator of two diagonal X-operators,

$$G_0^{a_1 a_1, a_2 a_2}(\tau_1, \tau_2) = \delta_{a_1 a_2} x_{a_1} - x_{a_1} x_{a_2}.$$
 (B37)

It is independent of time because the diagonal X-operators do not have any dynamics in the atomic limit. In frequency space it is convenient to factor our the frequency-conserving δ -function, defining

$$\tilde{G}_0^{a_1b_1,a_2b_2}(\omega_1,\omega_2) = \beta \delta_{\omega_1+\omega_2,0} G_0^{a_1b_1,a_2b_2}(\omega_1), \quad (B38)$$

with

$$G_0^{a_1b_1, a_2b_2}(\omega_1) = \delta_{a_1b_2}\delta_{b_1a_2} \frac{x_{b_1} - \zeta x_{a_1}}{i\omega_1 - \epsilon_{a_1b_1}}.$$
 (B39)

As a simple check, let us use the above results to calculate the time-ordered electronic single-particle Green function,

$$G_{\sigma}(\tau - \tau') = -\langle \mathcal{T}\hat{c}_{\sigma}(\tau)\hat{c}_{\sigma}^{\dagger}(\tau')\rangle$$
$$= -\frac{1}{\mathcal{Z}} \operatorname{tr} \left[e^{-\beta \hat{H}} \mathcal{T} \left\{ \hat{c}_{\sigma}(\tau)\hat{c}_{\sigma}^{\dagger}(\tau') \right\} \right]. \quad (B40)$$

Using Eq. (3.4) to express the canonical annihilation and creation operators in terms of X-operators we obtain in frequency space

$$G_{\sigma}(\omega) = G_0^{0\sigma,\sigma_0}(\omega) + G_0^{\bar{\sigma}2,2\bar{\sigma}}(\omega)$$

$$= \frac{x_0 + x_{\sigma}}{i\omega + \epsilon_0 - \epsilon_{\sigma}} + \frac{x_{\bar{\sigma}} + x_2}{i\omega + \epsilon_{\bar{\sigma}} - \epsilon_2}.$$
 (B41)

In the absence of a magnetic field we recover the well-known result 39 52

$$G(\omega) = \frac{1 - \frac{n}{2}}{i\omega + \mu} + \frac{\frac{n}{2}}{i\omega + \mu - U}$$
$$= \frac{\frac{1+x}{2}}{i\omega + \mu} + \frac{\frac{1-x}{2}}{i\omega + \mu - U}, \tag{B42}$$

where

$$n = \sum_{\sigma} \langle c_{\sigma}^{\dagger} c_{\sigma} \rangle = \sum_{\sigma} (x_{\sigma} + x_{2}) = x_{\uparrow} + x_{\downarrow} + 2x_{2} \quad (B43)$$

is the lattice filling (i.e., the average particle number per lattice site) and in the second line we have expressed the lattice filling in terms of the hole doping x=1-n. Note that a half-filled lattice corresponds to n=1 and $\mu=U/2$. In general, the lattice filling n and the hole doping x are related to the chemical potential via

$$n = 1 - x = \frac{2e^{\beta\mu} + 2e^{\beta(2\mu - U)}}{1 + 2e^{\beta\mu} + e^{\beta(2\mu - U)}}.$$
 (B44)

APPENDIX C: FERMIONIC FOUR-POINT VERTEX OF THE HUBBARD ATOM AT $U=\infty$

In this appendix we derive the expressions for the fermionic four-point vertex of the t model for vanish-

ing hopping given in Eqs. (5.43) and (5.44) of Sec. VB To derive the effective interaction between the projected fermions in the t model for vanishing hopping, we need the connected part of the four-point function of the projected fermionic annihilation and creation operators $\tilde{c}_{\sigma}(\tau) = X^{0\sigma}(\tau)$ and $\tilde{c}_{\sigma}^{\dagger}(\tau) = X^{\sigma 0}(\tau)$.

Let us introduce the following notation,

$$G_0^{\tilde{c}_{\sigma_1}\tilde{c}_{\sigma_2}\tilde{c}_{\sigma_1}^{\dagger}}(\tau_1, \tau_2; \tau_2', \tau_1') = \langle \mathcal{T} \left\{ \tilde{c}_{\sigma_1}^{\dagger}(\tau_1') \tilde{c}_{\sigma_2}^{\dagger}(\tau_2') \tilde{c}_{\sigma_2}(\tau_2) \tilde{c}_{\sigma_1}(\tau_1) \right\} \rangle_{\text{connected}}$$

$$= \langle \mathcal{T} \left\{ X^{\sigma_1 0}(\tau_1') X^{\sigma_2 0}(\tau_2') X^{0\sigma_2}(\tau_2) X^{0\sigma_1}(\tau_1) \right\} \rangle_{\text{connected}}$$

$$= \langle \mathcal{T} \left\{ X^{\sigma_1 0}(\tau_1') X^{\sigma_2 0}(\tau_2') X^{0\sigma_2}(\tau_2) X^{0\sigma_1}(\tau_1) \right\} \rangle$$

$$- \langle \mathcal{T} \left\{ X^{\sigma_1 0}(\tau_1') X^{0\sigma_1}(\tau_1) \right\} \rangle \langle \mathcal{T} \left\{ X^{\sigma_2 0}(\tau_2') X^{0\sigma_2}(\tau_2) \right\} \rangle$$

$$+ \langle \mathcal{T} \left\{ X^{\sigma_1 0}(\tau_1') X^{0\sigma_2}(\tau_2) \right\} \rangle \langle \mathcal{T} \left\{ X^{\sigma_2 0}(\tau_2') X^{0\sigma_1}(\tau_1) \right\} \rangle. \tag{C1}$$

We now employ Eqs. (A1) and (A6) to explicitly calculate the four-point function. For parallel spin $(\sigma_1 = \sigma_2 = \sigma)$, we obtain in frequency space,

$$\tilde{G}_{0}^{\tilde{c}_{\sigma}\tilde{c}_{\sigma}\tilde{c}_{\sigma}^{\dagger}\tilde{c}_{\sigma}^{\dagger}}(\omega_{1},\omega_{2};\omega_{2}',\omega_{1}') = \beta\delta_{\omega_{1}'+\omega_{2}',\omega_{2}+\omega_{1}}G_{0}^{\tilde{c}_{\sigma}\tilde{c}_{\sigma}\tilde{c}_{\sigma}^{\dagger}\tilde{c}_{\sigma}^{\dagger}}(\omega_{1},\omega_{2};\omega_{2}',\omega_{1}')$$

$$= \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} \int_{0}^{\beta} d\tau_{2}' \int_{0}^{\beta} d\tau_{1}' e^{i(\omega_{1}\tau_{1}+\omega_{2}\tau_{2}-\omega_{2}'\tau_{2}'-\omega_{1}'\tau_{1}')} \left\langle \mathcal{T}\left\{X^{\sigma 0}(\tau_{1}')X^{\sigma 0}(\tau_{2}')X^{0\sigma}(\tau_{2})X^{0\sigma}(\tau_{1})\right\}\right\rangle_{\text{connected}}$$

$$= \beta\delta_{\omega_{1}'+\omega_{2}',\omega_{2}+\omega_{1}} \left[\beta\delta_{\omega_{1}',\omega_{1}} - \beta\delta_{\omega_{2}',\omega_{1}}\right] \frac{n_{\bar{\sigma}}(1-n_{\bar{\sigma}})}{(i\omega_{1}'+\mu)(i\omega_{2}'+\mu)}.$$
(C2)

Actually, this expression is only valid for vanishing magnetic field so that we should set $n_{\uparrow} = n_{\downarrow} = n/2$. On the other hand, for the anti-parallel spin $(\sigma_2 = -\sigma_1 = -\sigma = \bar{\sigma})$, we obtain

$$\tilde{G}_{0}^{\tilde{c}_{\sigma}\tilde{c}_{\sigma}\tilde{c}_{\sigma}^{\dagger}\tilde{c}_{\sigma}^{\dagger}}(\omega_{1},\omega_{2};\omega'_{2},\omega'_{1}) = \beta\delta_{\omega'_{1}+\omega'_{2},\omega_{2}+\omega_{1}}G_{0}^{\tilde{c}_{\sigma}\tilde{c}_{\sigma}\tilde{c}_{\sigma}^{\dagger}\tilde{c}_{\sigma}^{\dagger}}(\omega_{1},\omega_{2};\omega'_{2},\omega'_{1})$$

$$= \int_{0}^{\beta} d\tau_{1} \int_{0}^{\beta} d\tau_{2} \int_{0}^{\beta} d\tau'_{2} \int_{0}^{\beta} d\tau'_{1} e^{i(\omega_{1}\tau_{1}+\omega_{2}\tau_{2}-\omega'_{2}\tau'_{2}-\omega'_{1}\tau'_{1})} \left\langle \mathcal{T}\left\{X^{\sigma 0}(\tau'_{1})X^{\bar{\sigma}0}(\tau'_{2})X^{0\bar{\sigma}}(\tau_{2})X^{0\bar{\sigma}}(\tau_{1})\right\}\right\rangle_{\text{connected}}$$

$$= \frac{\beta\delta_{\omega'_{1}+\omega'_{2},\omega_{2}+\omega_{1}}}{(i\omega'_{1}+\mu)(i\omega'_{2}+\mu)(i\omega_{1}+\mu)} \left\{ \left(1-\frac{n}{2}\right)(i\omega'_{1}+i\omega'_{2}+2\mu) - \left[\left(\frac{n^{2}}{4}-x_{2}\right)\beta\delta_{\omega'_{1},\omega_{1}}+\left(\frac{n}{2}-x_{2}\right)\beta\delta_{\omega'_{2},\omega_{1}}\right](i\omega_{1}+\mu)(i\omega_{2}+\mu)\right\}. \quad (C3)$$

The corresponding initial conditions of the four-point vertices are

$$\Gamma_0^{\bar{\psi}\bar{\psi}\psi\psi}(\omega_1'\sigma,\omega_2'\sigma;\omega_2\sigma,\omega_1\sigma) = -\left[\frac{(1-\frac{n}{2})^4}{(i\omega_1'+\mu)(i\omega_2'+\mu)(i\omega_2+\mu)(i\omega_1+\mu)}\right]^{-1}G_0^{\tilde{c}_\sigma\tilde{c}_\sigma\tilde{c}_\sigma^\dagger\tilde{c}_\sigma^\dagger}(\omega_1,\omega_2;\omega_2',\omega_1')$$

$$= -\beta(\delta_{\omega_1',\omega_1} - \delta_{\omega_2',\omega_1})\frac{\frac{n}{2}}{(1-\frac{n}{2})^3}(i\omega_1+\mu)(i\omega_2+\mu), \tag{C4}$$

and

$$\Gamma_{0}^{\bar{\psi}\bar{\psi}\psi\psi}(\omega'_{1}\sigma,\omega'_{2}\bar{\sigma};\omega_{2}\bar{\sigma},\omega_{1}\sigma) = -\left[\frac{(1-\frac{n}{2})^{4}}{(i\omega'_{1}+\mu)(i\omega'_{2}+\mu)(i\omega_{2}+\mu)(i\omega_{1}+\mu)}\right]^{-1}G_{0}^{\tilde{c}_{\sigma}\tilde{c}_{\bar{\sigma}}^{\dagger}\tilde{c}_{\bar{\sigma}}^{\dagger}}(\omega_{1},\omega_{2};\omega'_{2},\omega'_{1})$$

$$= -\frac{i\omega'_{1}+i\omega'_{2}+2\mu}{(1-\frac{n}{2})^{3}} + \frac{\beta}{(1-\frac{n}{2})^{4}}\left[\left(\frac{n^{2}}{4}-x_{2}\right)\delta_{\omega'_{1},\omega_{1}} + \left(\frac{n}{2}-x_{2}\right)\delta_{\omega'_{2},\omega_{1}}\right](i\omega_{1}+\mu)(i\omega_{2}+\mu).$$
(C5)

For the special frequency combination needed in the FRG flow equation (5.41), this reduces to

$$\Gamma_0^{\bar{\psi}\bar{\psi}\psi\psi}(\omega\sigma,\omega'\sigma;\omega'\sigma,\omega\sigma) = -\frac{\beta\frac{n}{2}}{(1-\frac{n}{2})^3}(1-\delta_{\omega,\omega'})(i\omega+\mu)(i\omega'+\mu),\tag{C6}$$

and

$$\Gamma_0^{\bar{\psi}\bar{\psi}\psi\psi}(\omega\sigma,\omega'\bar{\sigma};\omega'\bar{\sigma},\omega\sigma) = -\frac{i\omega + i\omega' + 2\mu}{(1-\frac{n}{2})^3} + \frac{\beta}{(1-\frac{n}{2})^4} \left[\left(\frac{n^2}{4} - x_2\right) + \left(\frac{n}{2} - x_2\right) \delta_{\omega,\omega'} \right] (i\omega + \mu)(i\omega' + \mu). \tag{C7}$$

For $U = \infty$ where $x_2 = 0$ the four-point vertices (C6) and (C7) reduce to the expressions given in Eqs. (5.43) and (5.44) of the main text.

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