Extremely correlated Fermi liquids: The formalism

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We present the detailed formalism of the extremely correlated Fermi liquid theory, developed for treating the physics of the t-J model. We start from the exact Schwinger equation of motion for the Green's function for projected electrons, and develop a systematic expansion in a parameter λ, relating to the double occupancy. The resulting Green's function has a canonical part arising from an effective Hamiltonian of the auxiliary electrons, and a caparison part playing the role of a frequency-dependent adaptive spectral weight. This adaptive weight balances the requirement at low ω of the invariance of the Fermi volume, and at high ω of decaying as $\frac{c_0}{i\omega}$, with a correlation-depleted $c_0 < 1$. The effective Hamiltonian H_{eff} describing the auxiliary fermions is given a natural interpretation with an effective interaction V_{eff} containing both the exchange J_{ij} and the hopping parameters t_{ij}. It is made Hermitian by adding suitable terms that ultimately vanish, in the *symmetrized theory* developed in this paper. Simple but important *shift invariances* of the t-J model are noted with respect to translating its parameters uniformly. These play a crucial role in constraining the form of V_{eff} and also provide checks for further approximations. The auxiliary and physical Green's function satisfy two sum rules, and the Lagrange multipliers for these are identified. A complete set of expressions for the Green's functions to second order in λ is given, satisfying various invariances. A systematic iterative procedure for higher order approximations is detailed. A superconducting instability of the theory is noted at the simplest level with a high transition temperature.

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I. INTRODUCTION

This work presents the detailed formalism of a newly developed framework for systematic calculation of the dynamical properties of the t-J model, starting from the basic parameters t and J of the model. A subsequent paper Ref. 1 presents self-consistent numerical results from the initial application of this theory, for the case of a two-dimensional square lattice relevant to cuprate superconductors. We will refer to *extreme correlations* as the limit $U \gg t$, so that the single-occupancy constraint is enforced. The t-J model Eq. (12) is the prime example of such a situation. In practice this theory applies already when $U \gtrapprox Zt$, where Z is the coordination number of the lattice. The theory and calculations presented are in the *extremely correlated Fermi liquid* (ECFL) phase discussed in Ref. 2. This phase is liquid like, and connects continuously to the Fermi liquid phase of weak-coupling models such as the Hubbard model, while accommodating the extreme local interaction $U \to \infty$.

The t-J model described by Eq. (12) is one of the standard models of condensed matter physics. It has been the focus of intense effort for the last few decades, as reviewed in Ref. 3. Interest in the model grew particularly after its identification by Anderson in Ref. 4, as governing many of the rich and complex set of phenomena in high-T_c cuprate superconductors. The origin of the exchange part of the t-J model in an inverse expansion in the interaction U is familiar from superexchange theory. The relation $J = \frac{4t^2}{U}$ is found starting from the Hubbard model as in Ref. 5, so that large U leads to a small J. An early account of the model and the various sum rules can be found in the Ref. 5. More recently Zhang and Rice[6] gave an argument for reducing the three-band copper oxygen model to an effective single-band model, with a t-J form. Their method, apart from being more realistic, gives independent magnitudes for t and J unconstrained by relations of the type inherent in superexchange within a single-band model.

Controlled calculations within this model are beset by two fundamental difficulties: (a) the noncanonical nature of the single-occupancy (Gutzwiller[7]) projection of the electrons that changes the canonical anticommutation relations to a more nontrivial Hubbard (Lie) algebra and (b) the absence of any obvious small parameter for generating a systematic theory. The present author has recently formulated a method in Ref. 2 and Ref. 8 that overcomes these difficulties to a large extent. The basic idea is to approach the system starting from the limit of low particle density $n = N_e/N_s$ (ratio of electron number to the number of sites), i.e., a generalized virial expansion. The density can be increased towards half filling systematically, as described below. Early applications to angle-resolved photoemission (ARPES) experiments in Ref. 9 are promising, and the general structure of the solution already leads to nontrivial and experimentally testable predictions in Ref. 10. The present work gives the details of the method introduced in Ref. 2, and carries out a calculation to the lowest nontrivial order in a parameter λ described below. The main elements involved in this framework can be summarized as follows:

(1) *The Schwinger method*. Reference 2 utilizes the key observation that the Schwinger method dispenses with Wicks theorem, and replaces that step of canonical theory by a formal matrix (operator) inversion. The Schwinger equation for the Green's function typically involves a time derivative and a functional derivative with respect to a source potential $\mathcal{V}$ (defined more fully below). It has the great advantage over standard equations of motion in that the functional derivative generates all required higher order Green's functions. This is unlike, say, the BBGKY hierarchy of quantum statistical mechanics, where one needs to import higher order correlations from elsewhere. For the t-J model, Ref. 2 obtains an exact Schwinger equation described below in Eq. (42) and Eq. (43). For our purpose, that equation may be illustrated schematically

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by the symbolic equation

$$\left[\hat{G}_0^{-1}(\boldsymbol{\mu}) - Y_1 - X\right] \cdot \mathcal{G} = (\mathbb{1} - \gamma), \tag{1}$$

where $\hat{G}_0^{-1}$ [Eq. (64)] is a noninteracting Green's function and γ [Eq. (35)] is essentially the spatially localized but time-dependent Green's function itself $\sim \mathcal{G}_{\text{local}}$. Further, Y_1 is a Hartree-type energy and $X \sim$ (something) $\times \frac{\delta}{\delta \mathcal{V}}$ contains the all-important functional derivative with respect to $\mathcal{V}$ [both X, Y are defined in Eq. (43)]. The undefined "something" lumps together constants and the interaction potential, but is independent of $\mathcal{G}$. This is a convenient launching pad provided by Schwinger's method, since it is exact. However, it is also intractable as it stands. There is no obvious small parameter, and the presence of the time-dependent γ on the right-hand side represents the removal of states (and double occupancy) from the canonical theory and creates a new set of problems. We must understand and overcome these in order to create a practical and controlled scheme for calculations. We therefore push forward to the next set of steps.

(2) *Noncanonical nature of the problem and its consequences*. The noncanonical nature of the problem is reflected in the γ term on the right of Eq. (1); it is a time-dependent Green's function obtainable from $\mathcal{G}$ itself [Eq. (45)]. This γ term contains an essential difficulty of the problem; it has a technical origin that we first discuss, and also an important physical aspect that we describe below.

(a) Consider first the canonical theories, such as the Hubbard model [see Eq. (4) below], where one only has the $\mathbb{1}$ term on the right-hand side of Eq. (1). In order to get rid of the functional derivative operator X in favor of a (multiplicative) self-energy, one uses $X \sim$ (something) $\times \frac{\delta}{\delta \mathcal{V}}$ to write

$$\begin{aligned} X \cdot \mathcal{G} &\to \Sigma \mathcal{G} \equiv (\text{something}) \times \mathcal{G}\Gamma\mathcal{G}, \\ \text{using } \frac{\delta}{\delta \mathcal{V}}\mathcal{G} &= \mathcal{G}\Gamma\mathcal{G}, \\ \text{following from } \Gamma &\equiv -\frac{\delta}{\delta \mathcal{V}}\mathcal{G}^{-1}, \end{aligned} \tag{2}$$

wherein the vertex Γ is introduced. This gives the Schwinger-Dyson relationship between the self-energy Σ and vertex:

$$\Sigma = (\text{something}) \times \mathcal{G}\Gamma, \quad \text{so that} \quad \left(\hat{G}_0^{-1}(\boldsymbol{\mu}) - Y_1 - \Sigma\right)\mathcal{G} = \mathbb{1}. \tag{3}$$

This Schwinger-Dyson construction necessarily requires that the vertex Γ reduce to unity at high frequencies, i.e., should be "asymptotically free." In the case of the noncanonical theory Eq. (1), a similar procedure fails. It is easily verified that the required good behavior is lost because of the time-dependent term γ on the right-hand side of Eq. (1), as shown in Ref. 11. The so defined vertex grows linearly with frequency, and invalidates the Dysonian self-energy scheme.

(b) The physical problem that is related to the noncanonical γ term has to do with the spectral weight of the projected electrons in a t-J model. Here basic sum rules give us insight into the origin, as well as a resolution of this fundamental problem. For noncanonical electrons, the high-frequency behavior of the Green's function is $\mathcal{G} \sim \frac{c_0}{i\omega}$ with $c_0 = 1 - \frac{n}{2}$, rather than the familiar result for canonical electrons $c_0 = 1$. The depletion of c_0 from unity arises from the physics of single-occupancy projection of the (noncanonical) electrons $\hat{c}_{i\sigma}$ (denoted by the Hubbard operator $X_i^{\sigma 0}$ below). Consider the relation $c_0 = \langle \hat{c}_{i\sigma}\hat{c}_{i\sigma}^\dagger + \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}\rangle$; the process $\langle \hat{c}_{i\sigma}\hat{c}_{i\sigma}^\dagger\rangle$ suffers from the inhibiting requirement that in order to create an electron with spin σ, the spin state $\bar{\sigma}$ at site i must also be unoccupied (so that a double occupancy is not created by this process), resulting in $c_0 < 1$. On the other hand, if the numerator of $\mathcal{G}(i\omega)$ remains as c_0 *at all frequencies*, then the Fermi surface must enlarge in volume, and thereby violate the Luttinger-Ward theorem of invariance of this volume.[12] We thus arrive at an appreciation of the fundamental tension between the conflicting requirements: at high frequency of fixing a known coefficient $c_0 < 1$, and at low frequency of a numerator almost unshifted from unity, for preserving the Fermi surface volume. A resolution is provided by the possibility of an adaptive (or smart) spectral weight, i.e., the numerator of the Green's function. If a frequency-dependent spectral weight can be found, so as to interpolate smoothly between the high- and low-frequency requirements, then both could be satisfied.

(c) The product ansatz: The above points suggest that the Green's function of the t-J model is usefully thought of as a product of two terms in frequency space i.e., $\mathcal{G} \sim \mathbf{g} \times \mu$ [Eq. (44)], where $\mathbf{g}$ is a canonical Green's function and μ the caparison factor playing the role of an adaptive (or smart) spectral weight factor. The $\mathbf{g}$ term (i.e., the denominator) is required to be a canonical object with its poles and cuts as usual in a Fermi liquid, and defines the auxiliary Fermi liquid in this theory. The frequency-dependent μ term (in the numerator) plays the role of the smart spectral weight; it reduces to the correct coefficient c_0 at high frequencies while recovering weight at lower frequencies. Thus a convolution in time domain into two suitable time-dependent pieces could resolve this conundrum, and motivates the *product ansatz* in Eq. (44). This *product ansatz* is at the heart of the procedure described here and is seen to lead to a pair of *exact* equations for the two parts $\mathbf{g}$ and μ below in Eq. (67) and Eq. (68).

(d) The μ term is also termed the caparison factor in Ref. 2, keeping in mind that it provides a second layer of dressing, over and above the dressing provided by the usual Fermi-liquid-type processes in $\mathbf{g}$ itself.

(3) *Small parameter in theory*. The t-J model is the sum of two highly nontrivial terms, the kinetic energy projected to the space of single occupancy, and the exchange energy. It has no obvious small parameters making it especially difficult to deal with. Some inspiration is gained by examining the form of the analogous Schwinger equation for canonical theories, such as the Hubbard model. Again omitting details, the relevant equation can be written symbolically as

$$\left[\hat{G}_0^{-1}(\boldsymbol{\mu}) - UG - U\frac{\delta}{\delta \mathcal{V}}\right] \cdot G = \mathbb{1}, \tag{4}$$

where U is the Coulomb repulsion in the Hubbard model. Comparing with Eq. (1) suggests a simple approach to introduce a new parameter λ. In its simplest form, we propose to study the modified problem symbolically expressed as

$$\left[\hat{G}_0^{-1}(\boldsymbol{\mu}) - \lambda Y_1 - \lambda X\right] \cdot \mathcal{G} = (\mathbb{1} - \lambda\gamma), \tag{5}$$

with $0 \leqslant \lambda \leqslant 1$, so that this equation Eq. (5) interpolates smoothly between the Fermi gas and the t-J model. This appearance of the parameter parallels the way the Hubbard parameter U enters Eq. (4). The complication of the noncanonical γ term on the right is handled analogously to the Hartree term Y_1. Unlike the repulsive Hubbard case, with an infinite interval $[0,\infty]$ for U, the parameter λ lives in a small and finite interval $[0,1]$. The expectation is that low-order perturbation expansion in λ has a reasonable chance of capturing the physics of extreme correlations at $\lambda = 1$. We show in Appendix A that in the atomic limit, the role of λ can be explicitly related to that of the fraction of double occupancy (and thus also density), so that tuning λ smoothly adjusts this fraction between its two limits. Further in Eq. (11) below, a suggestive expression for the fermionic operators is noted that relates $\lambda < 1$ to a soft version of Gutzwiller projection.

(4) *Effective Hamiltonian for the auxiliary fermions with a pseudopotential*. Setting aside the caparison factor μ for a moment, we examine further the equations of motion [Eq. (22) and Eq. (26)] for the auxiliary fermion $\mathbf{g}$ following from Eq. (5) together with the product ansatz $\mathcal{G} = \mathbf{g} \times \mu$. We would like to interpret these as the actual (canonical) equations of a suitable Fermi liquid, obtainable from a Hermitian Hamiltonian. However, we find that the equations [Eq. (22) and Eq. (26)] as they stand do not immediately cooperate with this task. They require a process of symmetrization described next, where one adds extra terms that vanish when treated exactly, and after this lead to a Hermitean theory for $\mathbf{g}$. We term the resulting equations as the *symmetrized theory*, as outlined in this paper.

The theory based on Eq. (22) and Eq. (26) without symmetrization is of course also exact, and is potentially useful in its own right. We develop such a *minimal theory* elsewhere, with the expectation that this *minimal theory* would not admit a Hermitian Hamiltonian to describe the auxiliary $\mathbf{g}$. Also in an approximate treatment, e.g., through an expansion in the parameter λ to any fixed but finite order, we would expect the symmetrized and minimal versions of the theory to be different, converging only when *all orders* are taken into account.

Returning to the symmetrization procedure, we construct an effective Hamiltonian H_{eff} for canonical electrons $(f_{i\sigma}, f_{i\sigma}^\dagger)$, with the property that the (imaginary time) Heisenberg equation of motion for canonical electrons $\dot{f}_{i\sigma} = -[f_{i\sigma}, H_{\text{eff}}]$ matches exactly the Heisenberg equation of motion for projected electrons $\dot{\hat{c}}_{i\sigma} = -[\hat{c}_{i\sigma}, H_{t-J}]$, except for terms that vanish on enforcing the single-occupancy constraint on the auxiliary $f_{i\sigma}$ electrons. Thus we require

$$[f_{i\sigma}, H_{\text{eff}}] = ([\hat{c}_{i\sigma}, H_{t-J}])_{(\hat{c},\hat{c}^\dagger)\to(f,f^\dagger)} + (\text{expressions involving } f, f^\dagger \text{ that vanish at single occupancy}). \tag{6}$$

We can then add these missing terms with $(f, f^\dagger) \to (\hat{c}, \hat{c}^\dagger)$ to the Heisenberg equation of motion (EOM) for $\hat{c}$ and thereby obtain an auxiliary Fermi liquid that would be also "natural," i.e., have all the standard properties of a Fermi liquid.[13,14] One should therefore be able to use standard Feynman diagrams (Ref. 13) to compute the properties of this auxiliary theory in powers of λ, if one were so inclined.

We find it straightforward to find such an effective Hamiltonian H_{eff} [Eq. (27)] as described below in Sec. II C. The physical meaning of H_{eff} becomes clearer with the following remarks. The kinetic energy of the projected electrons could also be written differently. An alternate representation, occasionally used in literature, relates

$$\hat{c}_{i\sigma}^\dagger = X_i^{\sigma 0} \to f_{i\sigma}^\dagger(1 - n_{i\bar{\sigma}}), \quad \hat{c}_{i\sigma} = X_i^{0\sigma} \to f_{i\sigma}(1 - n_{i\bar{\sigma}}) \tag{7}$$

with $\bar{\sigma} = -\sigma$ and $n_{i\sigma} = f_{i\sigma}^\dagger f_{i\sigma}$. Within this representation, the Hilbert space continues to allow for double occupancy, i.e., is canonical, but the various operators representing the physical processes act only upon the singly occupied subspace, *and produce states that are likewise singly occupied*. Thus we may write the kinetic energy part as

$$KE = -\sum_{ij} t_{ij}(1 - n_{i\bar{\sigma}}) f_{i\sigma}^\dagger f_{j\sigma}(1 - n_{j\bar{\sigma}}). \tag{8}$$

Since the exchange energy $\sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$ automatically conserves single occupancy, we will not write it out. The kinetic energy is thus a multi-Fermi operator and represents both the propagation and interaction between particles. To separate these functionalities, we introduce a parameter λ here—it will turn out to be the same parameter as in Eq. (5)—and write

$$\begin{aligned} KE(\lambda) &= -\sum_{ij} t_{ij}(1 - \lambda n_{i\bar{\sigma}}) f_{i\sigma}^\dagger f_{j\sigma}(1 - \lambda n_{j\bar{\sigma}}) \\ &= -\sum_{ij} t_{ij} f_{i\sigma}^\dagger f_{j\sigma} + \lambda \sum_{ij} t_{ij}\, f_{i\sigma}^\dagger f_{j\sigma}(n_{i\bar{\sigma}} + n_{j\bar{\sigma}}) \\ &\quad + \lambda^2 H_d, \end{aligned} \tag{9}$$

$$H_d = -\sum_{ij} t_{ij}\, f_{i\sigma}^\dagger f_{j\sigma}(n_{i\bar{\sigma}} n_{j\bar{\sigma}}), \quad H_d \to \text{dropped}. \tag{10}$$

The term H_d acts on the doubly occupied subspace and is null in the singly occupied space, and hence it may be dropped altogether. The remaining part of the kinetic energy term $KE(\lambda)$ has the structure of a four-Fermi interaction between the canonical fermions, and turns out to be a large part of H_{eff} in Eq. (27). The introduction of the parameter λ can thus be viewed as replacing Eq. (7) by a "softer" representation of the Gutzwiller projection:

$$\hat{c}_{i\sigma}^\dagger \to f_{i\sigma}^\dagger(1 - \lambda n_{i\bar{\sigma}}), \quad \hat{c}_{i\sigma} \to f_{i\sigma}(1 - \lambda n_{i\bar{\sigma}}). \tag{11}$$

This λ representation discourages but does not completely eliminate double occupancy. However as $\lambda \to 1$, it does become the exact projected operators Eq. (7), and further provides a simple interpolation between standard (canonical) fermions and the projected electrons by varying λ in the range $0 \leqslant \lambda \leqslant 1$. Thus Eq. (11) suggests the interpretation of the parameter λ as the controller of the (partial) Gutzwiller projection.

In this representation (with $\lambda = 1$), the physical electron Green's function $\mathcal{G}_{ij}$ corresponds to the correlator $-\langle\langle (1 - n_{i\bar{\sigma}_i}) f_{i\sigma_i}, f_{j\sigma_j}^\dagger (1 - n_{i\bar{\sigma}_j}) \rangle\rangle$, while $-\langle\langle f_{i\sigma_i}, f_{j\sigma_j}^\dagger \rangle\rangle$ would represent

the auxiliary Green's function $\mathbf{g}(i,j)$. The caparison factor μ seems hard to interpret in this language, though. The ECFL formalism developed here presents a procedure to splice together $\mathbf{g}$ and μ precisely, to yield the physical $\mathcal{G}$. Its otherwise formal structure becomes clearer upon making the above connection; in particular Eq. (11) helps in developing some intuition for $\mathbf{g}$. For instance a physical interpretation of the auxiliary fermions is provided by the $f_{i\sigma}$ themselves, and thereby requiring the same number of auxiliary fermions as the physical ones, as done below, is perfectly natural.

(5) *Invariances of the effective Hamiltonian $H_{\rm eff}$ and the emergence of the second chemical potential u_0.* In $H_{\rm eff}$ [Eq. (27)], the hopping parameter t_{ij} is elevated to the role of an interaction coupling, in addition to its role as a band-hopping parameter. This feature needs attention, since we know that a constant (k independent) shift of the band energies $\varepsilon_k \to \varepsilon_k + u_t$, or adding an on-site interaction through $J_{ij} \to J_{ij} + \delta_{ij} u_J$, is inconsequential for the t-J model, but makes a difference in Eq. (9), and in various approximations for the t-J model. This "pure" gauge invariance is of primary importance in this kind of a theory, and must be addressed at the very outset to obtain a consistent and meaningful description of the t-J model. Such shifts could potentially lead to a change of the interaction strengths in $H_{\rm eff}$, unless they can be explicitly eliminated in the theory. This issue is addressed by first listing these *shift symmetries* of the model in Sec. II, and then requiring the approximation scheme to be shift invariant, at each order of λ.

Imposing the shift symmetries on $H_{\rm eff}$ Eq. (27) causes it to have a term with a Hubbard-Coulomb-like interaction with strength u_0, such that arbitrary shifts of t and J can be absorbed into the parameter u_0. Analogous to the standard chemical potential $\boldsymbol{\mu}$, this u_0 is a Lagrange multiplier of a term in the Hamiltonian $H_{\rm eff}$. However it multiplies an interaction term that is *quartic* in the canonical fermions, unlike $\boldsymbol{\mu}$ that multiplies the usual (quadratic) number operator. The chemical potential $\boldsymbol{\mu}$ and the second chemical potential u_0 are jointly determined by *two sum rules* Eq. (90) and Eq. (91), one for the number of physical electrons and the other for the (identical) number of auxiliary canonical electrons.

In this work, we obtain a set of equations for the Green's function. These are essentially of the same form as in our recent earlier Letter Ref. 2, but differ in a few details due to the usage of the idea of the effective Hamiltonian and its shift invariances. An iterative framework is carefully established, and calculations of the Green's function to second order in λ are carried out explicitly.

The outline of the paper is as follows. In Sec. II, we list the *shift symmetries* of the t-J model and obtain the exact equation satisfied by the Green's function. We also determine the form of the effective Hamiltonian $H_{\rm eff}$ for the auxiliary fermions, such that the Heisenberg equations for the field operators are satisfied in a Hermitian framework. In Secs. III and IV, we use the *product ansatz* for the Green's function to introduce and find the exact equations for the auxiliary fermions and the caparison factor μ. In Sec. V we turn off the time-dependent sources and write the exact momentum-space relations between the self-energy, the caparison factor, and the physical Green's functions—these are the analogs of the Schwinger-Dyson equations for this problem. Section VI summarizes in tabular form the necessary equations needed for the next step in the iterative process that is analogous to the skeleton graph expansion. Section VII describes the λ expansion of various objects and the precise nature of the iterative expansion. Several detailed calculations are needed to obtain the second-order equations, and are detailed in Appendix B. Section VIII details the Ward identities of this theory, which splits into two parts following the splitting of the Green's functions. Section IX gives the set of vertices defining the random phase approximation for this theory and Sec. X gives the formal results for the charge and spin susceptibilities within RPA and its low-order expansion. Section XI concludes with some comments including a calculation of the superconducting transition temperature in this theory.

Appendix A gives a detailed calculation in the atomic limit. The simple calculation here may be useful in providing the reader some insight into the interpretation of the λ expansion in terms of the number of doubly occupied sites. Appendix B contains the detailed calculations of the various objects need to compile the second-order Green's function.

II. THE t-J MODEL AND ITS SHIFT INVARIANCE

We write the projected Fermi operators in terms of the Hubbard X operators as usual $\hat{c}_{i\sigma} \to X_i^{0\sigma}$, $\hat{c}_{i\sigma}^\dagger \to X_i^{\sigma 0}$, and $\hat{c}_{i\sigma'}^\dagger \hat{c}_{i\sigma} \to X_i^{\sigma'\sigma}$. We study the t-J model given by

$$\begin{aligned} H &= -\sum_{i,j,\sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma} - \boldsymbol{\mu} \sum_{i,\sigma} X_i^{\sigma\sigma} \\ &\quad + \frac{1}{2}\sum_{i,j} J_{ij} \left\{ \vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right\}, \\ &= -\sum_{i,j,\sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma} - \boldsymbol{\mu} \sum_{i,\sigma} X_i^{\sigma\sigma} \\ &\quad + \frac{1}{4}\sum_{ij,\sigma} J_{ij} \left(X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} - X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}} \right). \end{aligned} \tag{12}$$

We will treat the two terms on an equal footing as far as possible, and allow terms with $i = j$. The statement of the model is invariant under a particular "pure gauge" transformation that we next discuss. Let us first note the *shift invariance* of the two parameters in H. Consider the uniform (i.e., space independent) shifts of the basic parameters:

$$t_{ij} \to t_{ij} - u_t \delta_{ij}, \quad J_{ij} \to J_{ij} + u_J \delta_{ij}, \tag{13}$$

with independent parameters u_t, u_J. Under this transformation the Hamiltonian shifts as

$$H \to H + \left(u_t + \tfrac{1}{4} u_J\right) \hat{N}, \tag{14}$$

where $\hat{N} = \sum_{i\sigma} X_i^{\sigma\sigma}$ is the number operator for the electrons. Let us note two simple theorems encoding this invariance:

Shift theorem I. A shift of either t or J can be absorbed into suitable parameters, leaving the physics unchanged.

Shift theorem II. The two shifts of t and J cancel each other when $u_J = -4u_t$.

The first theorem is illustrated in the initial Hamiltonian Eq. (12), where the shift in Eq. (14) can be absorbed in the chemical potential $\boldsymbol{\mu} \to \boldsymbol{\mu} + u_t + \frac{1}{4} u_J$. Later it serves to identify a second generalized chemical potential u_0 encountered

in the following. The second theorem is subtle as it leaves the chemical potential $\boldsymbol{\mu}$ unchanged (see Ref. 15). It provides a measure of the equal-handed treatment of t and J. We will find these almost trivial theorems of great use in devising and validating various approximation schemes later.

In further work we need to add a source term via the operator $\mathcal{A}$:

$$\mathcal{A} = \int_0^\beta \mathcal{A}(\tau)d\tau = \sum_{j,\sigma_1,\sigma_2} \int_0^\beta d\tau\ \mathcal{V}_j^{\sigma_1\sigma_2}(\tau)X_j^{\sigma_1\sigma_2}(\tau) + \sum_{ij,\sigma_1\sigma_2} \int_0^\beta d\tau\ \mathcal{V}_{ij}^{\sigma_1\sigma_2}(\tau)X_i^{\sigma_1 0}(\tau)X_j^{0\sigma_2}(\tau), \tag{15}$$

with the usual imaginary-time Heisenberg picture τ dependence of the operators $Q(\tau) = e^{\tau H}Qe^{-\tau H}$, and the bosonic sources $\mathcal{V}_j^{\sigma_1\sigma_2}(\tau)$ at every site and also $\mathcal{V}_{ij}^{\sigma_1\sigma_2}(\tau)$ for every pair of sites, as arbitrary functions of time. We will denote these sources in a compact notation where the site index also carries the time argument as $\mathcal{V}_i^{\sigma_1\sigma_2} \equiv \mathcal{V}_i^{\sigma_1\sigma_2}(\tau_i)$ and $\mathcal{V}_{ij}^{\sigma_1\sigma_2} \equiv \mathcal{V}_{ij}^{\sigma_1\sigma_2}(\tau_i)\delta(\tau_i - \tau_j)$. For any variable we define a modified expectation

$$\langle\langle Q(\tau_1,\tau_2,\ldots)\rangle\rangle = \frac{\mathrm{Tr}[e^{-\beta H}T_\tau e^{-\mathcal{A}}\ Q(\tau_1,\tau_2,..)]}{\mathrm{Tr}[e^{-\beta H}T_\tau(e^{-\mathcal{A}})]}, \tag{16}$$

with a compact notation that includes the (imaginary) time ordering symbol T_τ and the exponential factor automatically. With the abbreviation $i \equiv (R_i,\tau_i)$ for spatial $\vec{R}_i$ and imaginary-time (τ) coordinates, the physical electron is described by a Green's function:

$$\mathcal{G}_{\sigma_i\sigma_f}[i,f] = -\langle\langle X_i^{0\sigma_i}\ X_f^{\sigma_f 0}\rangle\rangle. \tag{17}$$

From this, the variation can be found from functional differentiation as

$$\frac{\delta}{\delta\mathcal{V}_j^{\sigma_1\sigma_2}(\tau_1)}\langle\langle Q(\tau_2)\rangle\rangle = \langle\langle Q(\tau_2)\rangle\rangle\langle\langle X_j^{\sigma_1\sigma_2}(\tau_1)\rangle\rangle - \langle\langle X_j^{\sigma_1\sigma_2}(\tau_1)Q(\tau_2)\rangle\rangle. \tag{18}$$

We note the fundamental anticommutator between the destruction and creation operators:

$$\left\{X_i^{0\sigma_1}, X_j^{\sigma_2 0}\right\} = \delta_{ij}\left(\delta_{\sigma_1\sigma_2} - (\sigma_1\sigma_2)X_i^{\bar{\sigma}_1\bar{\sigma}_2}\right). \tag{19}$$

A. The Heisenberg equation of motion

Let us now study the time evolution of the destruction operator through its important commutator:

$$\left[X_i^{0\sigma_i}, H\right] = -\sum_j t_{ij}\left[\delta_{\sigma_i\sigma_j} - (\sigma_i\sigma_j)X_i^{\bar{\sigma}_i\bar{\sigma}_j}\right]X_j^{0\sigma_j} \underbrace{+\frac{1}{4}J_0X_i^{0\sigma_i}} - \boldsymbol{\mu}X_i^{0\sigma_i} - \frac{1}{2}\sum_{j\neq i} J_{ij}(\sigma_i\sigma_j)X_j^{\bar{\sigma}_i\bar{\sigma}_j}X_i^{0\sigma_j}. \tag{20}$$

Here J_0 is the zero wave vector (i.e., J_{ii} the on-site) exchange constant. The term in underbraces here and in the next equation ensures that the commutator reproduces the term with $J_{ij} \to J_{ij} + u_J\delta_{ij}$ correctly. We note that under the transformation Eq. (14), the last term in Eq. (20) adds nothing, in view of the ordering of the operators as written, while the term with underbraces provides the correct transformation factor. Let us call this commutator

$$\left[X_i^{0\sigma_i}, H\right] = -\sum_j t_{ij}X_j^{0\sigma_i} \underbrace{+\frac{1}{4}J_0X_i^{0\sigma_i}} - \boldsymbol{\mu}X_i^{0\sigma_i} + A_{i\sigma_i}, \tag{21}$$

$$A_{i,\sigma_i} = \sum_{j\sigma_j} t_{ij}(\sigma_i\sigma_j)X_i^{\bar{\sigma}_i\bar{\sigma}_j}X_j^{0\sigma_j} - \frac{1}{2}\sum_{j\neq i} J_{ij}(\sigma_i\sigma_j)X_j^{\bar{\sigma}_i\bar{\sigma}_j}X_i^{0\sigma_j}. \tag{22}$$

We next express the EOM for the Green's function in terms of A.

B. Equation of motion for $\mathcal{G}$

Let us compute the time derivative of $\mathcal{G}$. For this we need the derivative

$$\begin{aligned}
\partial_{\tau_i}T_\tau\left(e^{-\mathcal{A}}X_i^{0\sigma_i}(\tau_i)\right) &= -T_\tau\left(e^{-\mathcal{A}}\left[X_i^{0\sigma_i}(\tau_i), H\right]\right) + T_\tau\left(e^{-\mathcal{A}}\left[\mathcal{A}(\tau_i), X_i^{0\sigma_i}(\tau_i)\right]\right),\\
\left[\mathcal{A}(\tau_i), X_i^{0\sigma_i}(\tau_i)\right] &= \mathcal{V}_i^{\sigma_1\sigma_2}(\tau_i)\left[X_i^{\sigma_1\sigma_2}(\tau_i), X_i^{0\sigma_i}(\tau_i)\right] - \sum_j \mathcal{V}_{ij}^{\sigma_1\sigma_2}(\tau_i)\left\{X_i^{\sigma_1 0}(\tau_i), X_i^{0\sigma_i}(\tau_i)\right\}X_j^{0\sigma_2}(\tau_i)\\
&= -\mathcal{V}_i^{\sigma_i\sigma_2}X_i^{0\sigma_2} - \sum_j \mathcal{V}_{ij}^{\sigma_i\sigma_2}X + j^{0\sigma_2} + \sum_j \mathcal{V}_{ij}^{\sigma_1\sigma_2}(\sigma_1\sigma_i)X_i^{\bar{\sigma}_i\bar{\sigma}_1}X_j^{0\sigma_2}.
\end{aligned} \tag{23}$$

This follows from the definition of the time ordering and Eq. (15) for $\mathcal{A}$. Using this we find

$$\begin{aligned}
\partial_{\tau_i}\mathcal{G}_{\sigma_i\sigma_f}[i,f] = &-\delta(\tau_i - \tau_f)\delta_{i,f}\langle\langle\left(\delta_{\sigma_i\sigma_f} - \sigma_i\sigma_f X_i^{\bar{\sigma}_i\bar{\sigma}_f}\right)\rangle\rangle + \langle\langle\left[X_i^{0\sigma_i}(\tau_i), H\right]X_f^{\sigma_f 0}(\tau_f)\rangle\rangle\\
&- \mathcal{V}_i^{\sigma_i\sigma_2}(\tau_i)\mathcal{G}_{\sigma_2\sigma_f}[i,f] - \sum_j \mathcal{V}_{ij}^{\sigma_i\sigma_2}\mathcal{G}_{\sigma_2\sigma_f}[j,f] - \sum_j \mathcal{V}_{ij}^{\sigma_1\sigma_2}(\sigma_1\sigma_i)\langle\langle X_i^{\bar{\sigma}_i\bar{\sigma}_1}(\tau_i)X_j^{0\sigma_2}(\tau_j)X_f^{\sigma_f 0}(\tau_f)\rangle\rangle.
\end{aligned} \tag{24}$$

To simplify notation, in such expressions for the Green's functions [or Eq. (26) below], the sum over an index implies a sum over the corresponding site and also an integration over the corresponding time; e.g., $\sum_j \mathcal{V}_{ij}^{\sigma_1\sigma_2}f(\ldots,\tau_j,\ldots) \to \sum_{R_j}\int_0^\beta d\tau_j\mathcal{V}_{ij}^{\sigma_1\sigma_2}(\tau_j)\delta(\tau_i - \tau_j)f(\ldots,\tau_j,\ldots)$. A further bold letter summation convention is used after Eq. (41). However, note that in expressions for operators such as Eq. (21) or Eq. (22), the sum only refers to the site index summation. We further

use the abbreviations

$$\delta[i,j] = \delta_{i,j}\ \delta(\tau_i - \tau_j), \quad t[i,j] = t_{ij}\ \delta(\tau_i - \tau_j),$$
$$J[i,j] = J_{ij}\ \delta(\tau_i - \tau_j) \quad \mathcal{V}_r^{\sigma_a\sigma_b} = \mathcal{V}_r^{\sigma_a\sigma_b}[\tau_r]. \tag{25}$$

In terms of these, and using Eq. (21), we find the equation of motion in terms of A:

$$(\partial_{\tau_i} - \boldsymbol{\mu})\mathcal{G}_{\sigma_i\sigma_f}[i,f] = -\delta[i,f]\langle\langle\delta_{\sigma_i,\sigma_f} - \sigma_i\sigma_f X_i^{\bar{\sigma}_i\bar{\sigma}_f}\rangle\rangle + t[i,j]\mathcal{G}_{\sigma_i\sigma_f}[j,f] - \frac{1}{4}J_0\mathcal{G}_{\sigma_i\sigma_f}[i,f] + \langle\langle A_{i\sigma_i}(\tau_i)X_f^{\sigma_f 0}(\tau_f)\rangle\rangle$$
$$- \mathcal{V}_i^{\sigma_i\sigma_j}(\tau_i) \quad \mathcal{G}_{\sigma_j\sigma_f}[i,f] - \sum_j \mathcal{V}_{ij}^{\sigma_i\sigma_2}\mathcal{G}_{\sigma_2\sigma_f}[j,f] - \sum_j \mathcal{V}_{ij}^{\sigma_1\sigma_2}(\sigma_1\sigma_i)\langle\langle X_i^{\bar{\sigma}_i\bar{\sigma}_1}(\tau_i)X_j^{0\sigma_2}(\tau_j)X_f^{\sigma_f 0}(\tau_f)\rangle\rangle. \tag{26}$$

We recall from the introduction the discussion regarding suitably generalizing A of Eq. (22), in order to make connection with a Hermitian H_{eff}, and therefore turn to this task next.

C. Effective Hamiltonian

We now construct an effective Hamiltonian of canonical fermions that will turn out to govern the auxiliary Fermi liquid theory. The motivation for this construction is to cast the auxiliary fermionic part of the ECFL theory into a natural and canonical framework, so that the equation for the $\mathbf{g}$, i.e., the auxiliary piece of the full $\mathcal{G}$, is obtainable from a Hamiltonian that is Hermitian and respects the usual Fermi symmetry of interactions under exchange.

After some inspections we find that a suitable Hamiltonian is provided by the expression

$$H_{\text{eff}} = -\sum_{ij} t_{ij} f_{i\sigma}^\dagger f_{j\sigma} + \sum_i \left(\frac{1}{4}J_0 - \mu\right) f_{i\sigma}^\dagger f_{i\sigma} + \lambda V_{\text{eff}},$$
$$V_{\text{eff}} = \frac{1}{4}\sum_{ij} t_{ij}(\sigma_1\sigma_2)\left[\left(f_{i\sigma_1}^\dagger f_{i\bar{\sigma}_1}^\dagger + f_{j\sigma_1}^\dagger f_{j\bar{\sigma}_1}^\dagger\right) f_{i\bar{\sigma}_2} f_{j\sigma_2} + (\text{H.c.})\right]$$
$$- \frac{1}{4}\sum_{ij} J_{ij}(\sigma_1\sigma_2) f_{i\sigma_1}^\dagger f_{j\bar{\sigma}_1}^\dagger f_{j\bar{\sigma}_2} f_{i\sigma_2}$$
$$+ \frac{1}{4}\sum_i u_0(\sigma_1\sigma_2) f_{i\sigma_1}^\dagger f_{i\bar{\sigma}_1}^\dagger f_{i\bar{\sigma}_2} f_{i\sigma_2}, \tag{27}$$

with a Hermitian effective potential $V_{\text{eff}}^\dagger = V_{\text{eff}}$ (Fig. 1), and assume no constraint on double occupancy for these auxiliary (canonical) fermions $f_{i\sigma}$. The t and J parts reproduce the exact equations of motion as shown below with certain additional terms that vanish under the constraint of single occupancy. The parameter λ is set to unity at the end and provides an interpolation to the Fermi gas. The parameter u_0 represent an effective Hubbard-type interaction for these fermions, giving a contribution $u_0 \sum_i f_{i\uparrow}^\dagger f_{i\uparrow} f_{i\downarrow}^\dagger f_{i\downarrow}$. Its magnitude is arbitrary at the moment, since it disappears under exclusion of double occupancy. Here it enables us to enforce the invariance in shift theorem I, where the shift of t and J can be absorbed in u_0. It will turn out to play the role of a second chemical potential or Lagrange multiplier, in fixing the second sum rule Eq. (91). To illustrate this remark, note that adding a constant to t or J as in Eq. (14) adds an on-site four-Fermi interaction term. In order to satisfy the shift theorem I, we must compensate for this suitably, leading to the extra on-site term with coefficient u_0, which can absorb this shift. It is also verified that the shift theorem II is satisfied without the u_0 term. We emphasize that the u_0 term is both natural and essential for the purpose of satisfying the shift theorem I. Since the structure of the u_0 term is almost identical to that of J_{ij} we will most often "hide it" inside J_{ij}, and explicitly display it at the end. Thus unless explicitly displayed, we should read $J_{ij} \to J_{ij} - u_0\delta_{ij}$ below. For analogous terms involving the $X_i^{\sigma\sigma'}$ operators as in Eq. (22), we can include u_0 in J_{ij} without any errors, since the u_0 term always vanishes due to the properties of these operators.

Defining symmetric Cooper pair singlet operators

$$\mathcal{P}^\dagger(i,j) = \sum \sigma f_{i\sigma}^\dagger f_{j\bar{\sigma}}^\dagger = (f_{i\uparrow}^\dagger f_{j\downarrow}^\dagger - f_{i\downarrow}^\dagger f_{j\uparrow}^\dagger),$$
$$\mathcal{P}^\dagger(i,i) = \sum \sigma f_{i\sigma}^\dagger f_{i\bar{\sigma}}^\dagger = 2 f_{i\uparrow}^\dagger f_{i\downarrow}^\dagger, \tag{28}$$

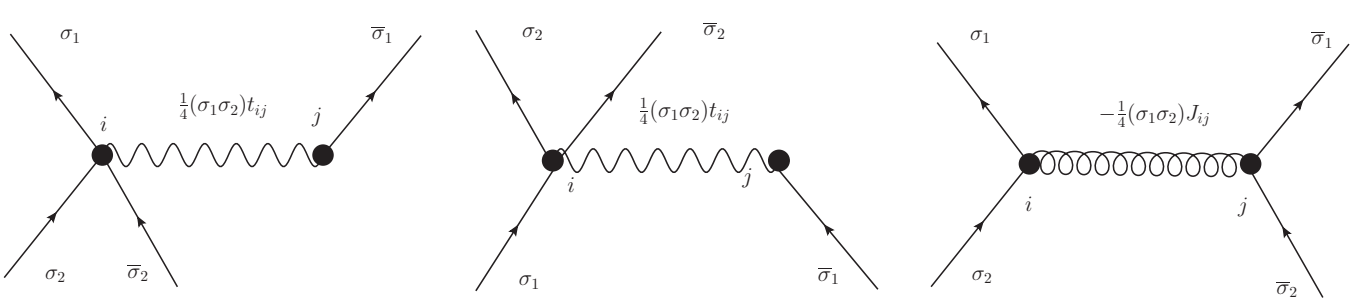
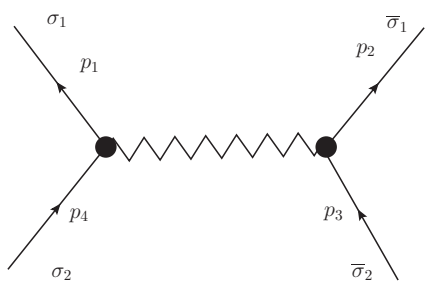


FIG. 1. The pseudopotential V_{eff} in the real-space representation, where the wavy line represents t_{ij} and the coiled line represents J_{ij}. The first two interaction vertices have two undisplayed symmetric partners with the exchange $i \leftrightarrow j$.



$W_{eff} = -\delta_{p_1+p_2,p_3+p_4} \ \{\Sigma_j \varepsilon_j + J_{p_2-p_3} - u_0\}$

FIG. 2. The pseudopotential $W_{\rm eff}$ in the momentum-space representation. The zigzag line represents $W_{\rm eff}$. Note that the momentum transfer in the argument of J is also expressible as $J_{p_1-p_4}$.

with $\mathcal{P}^\dagger(j,i) = \mathcal{P}^\dagger(i,j)$, we write

$$V_{\rm eff} = \frac{1}{4}\sum_{ij} t_{ij}[(\mathcal{P}^\dagger(i,i) + \mathcal{P}^\dagger(j,j))\mathcal{P}(i,j) + (\text{H.c.})] - \frac{1}{4}\sum_{ij} J_{ij}\mathcal{P}^\dagger_{ij}\mathcal{P}_{ij}. \tag{29}$$

In momentum representation the effective Hamiltonian Eq. (27) reads

$$\begin{aligned} H_{\rm eff} &= \sum_k \left(\varepsilon_k + \frac{1}{4}J_0 - \boldsymbol{\mu}\right) f^\dagger_{k\sigma} f_{k\sigma} \\ &\quad + \frac{\lambda}{4N_s}\sum_p (\sigma_1\sigma_2) W_{\rm eff}(p_1,p_2;p_3,p_4) \\ &\quad \times f^\dagger_{p_1\sigma_1} f^\dagger_{p_2\bar\sigma_1} f_{p_3\bar\sigma_2} f_{p_4\sigma_2}, \\ W_{\rm eff}(p_1,p_2;p_3,p_4) &= -\delta_{p_1+p_2,p_3+p_4}\{\varepsilon_{p_1} + \varepsilon_{p_2} + \varepsilon_{p_3} \\ &\quad + \varepsilon_{p_4} + J_{p_2-p_3} - u_0\} \end{aligned} \tag{30}$$

(see Fig. 2), where the momentum-independent term u_0 has been explicitly written out. In this effective Hamiltonian, the band energies ε_{p_j} of the original model are present, both in the band energy of the f's and the interaction term. Therefore the shift Eq. (13) cannot be absorbed in the $\boldsymbol{\mu}$ alone, and u_0 must also transform suitably to ensure that the effective Hamiltonian satisfies the shift theorem I. Thus in using the effective Hamiltonian we refine this theorem to

Shift theorem I.1. An arbitrary shift Eq. (14) of t and J can be absorbed by shifting the chemical potential $\boldsymbol{\mu} \to \boldsymbol{\mu} + u_t + \frac{1}{4}u_J$ and u_0 as

$$u_0 \to u_0 + 4u_t + u_J. \tag{31}$$

Note that the shift theorem II is manifestly satisfied: The combination of the band energies ε_{p_j} and the exchange term J_p in Eq. (30) guarantees that their shift adds up to $u_J + 4u_t \to 0$, which vanishes under the conditions of this theorem.

Since the standard notation for interaction reads $\sum\langle ab|V|a'b'\rangle f^\dagger_a f^\dagger_b f_{b'} f_{a'}$ for a conventional two-body interaction, our notation corresponds to writing $W_{\rm eff}(p_1,p_2;p_3,p_4) = \langle p_1p_2|W|p_4p_3\rangle$. Fermi symmetry implies the invariance $W_{\rm eff}(p_1,p_2;p_3,p_4) = W_{\rm eff}(p_2,p_1;p_4,p_3)$, and Hermiticity implies the invariance $W_{\rm eff}(p_1,p_2;p_3,p_4) = W_{\rm eff}(p_3,p_4;p_1,p_2)$. For this canonical theory, we calculate the commutator:

$$\begin{aligned} [f_{i\sigma_i}, H_{\rm eff}] &= -\sum_j t_{ij} f_{j\sigma_i} + \left(\frac{1}{4}J_0 - \boldsymbol{\mu}\right) f_{i\sigma_i} + \hat{A}_{i\sigma_i}, \\ \hat{A}_{i\sigma_i} &= [f_{i\sigma_i}, V_{\rm eff}], \end{aligned} \tag{32}$$

with

$$\begin{aligned} \hat{A}_{i\sigma_i} &= \sum_{j\sigma_j} t_{ij}(\sigma_i\sigma_j) \\ &\quad \times \left[f^\dagger_{i\bar\sigma_i} f_{i\bar\sigma_j} f_{j\sigma_j} \underbrace{+\frac{1}{2} f^\dagger_{j\bar\sigma_i} f_{j\bar\sigma_j} f_{j\sigma_j} + \frac{1}{2} f^\dagger_{j\bar\sigma_i} f_{i\bar\sigma_j} f_{i\sigma_j}} \right] \\ &\quad - \frac{1}{2}\sum_{j\neq i} J_{ij}(\sigma_i\sigma_j) f^\dagger_{j\bar\sigma_i} f_{j\bar\sigma_j} f_{i\sigma_j}. \end{aligned} \tag{33}$$

Let us note that $\hat{A}_{i\sigma}$ Eq. (33) differs from $A_{i\sigma}$ in Eq. (22), through terms (in underbraces) that vanish identically if we impose the single-occupancy constraint on the auxiliary electrons.

D. Equation of motion for $\mathcal{G}$ continued

We now return to the study of the equation of motion for $\mathcal{G}$ in Eq. (26), expressed in terms of $A_{i\sigma}$ of Eq. (22), the commutator of the destruction operator with H. This object yields the crucial Heisenberg equation of motion; therefore as discussed in Eq. (6), we next look for terms that can be added to it to make it identical to Eq. (33). Comparing Eq. (22) and Eq. (33) we see that these differ by terms [the second and third terms of the square bracket in Eq. (33)] that are automatically vanishing for the X_i^{ab} operators on using their standard rules. Thus we can add such vanishing terms to Eq. (22) that remain exact and also importantly preserve the Hermitian nature of the auxiliary fermionic theory in approximate schemes. We thus rewrite also an exact but more useful result:

$$\begin{aligned} A_{i,\sigma_i} &= \sum_{ij\sigma_j} t_{ij}(\sigma_i\sigma_j) \\ &\quad \times \left[X_i^{\bar\sigma_i\bar\sigma_j} X_j^{0\sigma_j} + \frac{1}{2} X_j^{\bar\sigma_i\bar\sigma_j} X_j^{0\sigma_j} + \frac{1}{2} X_j^{\bar\sigma_i 0} X_i^{0\bar\sigma_j} X_i^{0\sigma_j} \right] \\ &\quad - \frac{1}{2}\sum_{j\neq i} J_{ij}(\sigma_i\sigma_j) X_j^{\bar\sigma_i\bar\sigma_j} X_i^{0\sigma_j}, \end{aligned} \tag{34}$$

so that A_{i,σ_i} and $\hat{A}_{i,\sigma_i}$ contain terms that are in one to one correspondence. We will use Eq. (34) in in place of Eq. (22) in Eq. (26) next.

The notation simplifies if we use the matrix notation for the spin indices introduced in Ref. 11 and Ref. 2, e.g., $\mathcal{G}_{\sigma_i\sigma_f}[i,f] \to [\mathcal{G}[i,f]]_{\sigma_i\sigma_f}$, so that we may regard $\mathcal{G}$ as a 2×2 matrix. In short, the space-time indices are displayed but the spin indices are hidden in the above matrix structure. We next define γ through

$$\gamma_{\sigma_a\sigma_b}[i] = \sigma_a\sigma_b\mathcal{G}_{\bar\sigma_b\bar\sigma_a}[i^-,i], \quad \text{or} \quad \gamma[i] = \mathcal{G}^{(k)}[i^-,i], \tag{35}$$

where we denote the k conjugation of any matrix M by $(M^{(k)})_{\sigma_1\sigma_2} = M_{\bar\sigma_2\bar\sigma_1}\sigma_1\sigma_2$. This conjugation corresponds to time reversal in the spin space. Let $\mathbb{1}$ be the identity matrix in the 2×2 dimensional spin space.

We employ a useful relation with an arbitrary operator $\mathcal{Q}$ that follows from Eq. (16). We write

$$\begin{aligned}\langle\langle\sigma_a\sigma_b X_i^{\bar\sigma_a\bar\sigma_b}(\tau_i)\mathcal{Q}\rangle\rangle &= \left(\gamma_{\sigma_a\sigma_b}[i] - D_{\sigma_a\sigma_b}[i]\right)\langle\langle\mathcal{Q}\rangle\rangle,\\ \langle\langle\sigma_a\sigma_b X_i^{\bar\sigma_a 0}(\tau_i^+)X_j^{0\bar\sigma_b}(\tau_i)\mathcal{Q}\rangle\rangle &= \left(\gamma_{\sigma_a\sigma_b}[i,j] - D_{\sigma_a\sigma_b}[i,j]\right)\langle\langle\mathcal{Q}\rangle\rangle,\end{aligned} \tag{36}$$

where we set $\tau_j \to \tau_i^-$ and define

$$\gamma_{\sigma_a\sigma_b}[i,j] = (\sigma_a\sigma_b)\mathcal{G}_{\bar\sigma_b\bar\sigma_a}[j\tau_i^-,i\tau_i] = \langle\langle\sigma_a\sigma_b X_i^{\bar\sigma_a 0}X_j^{0\bar\sigma_b}\rangle\rangle, \tag{37}$$

$$\gamma[i,i] = \gamma[i], \tag{38}$$

and

$$\begin{aligned} D_{\sigma_i\sigma_j}[i] &= \sigma_i\sigma_j\frac{\delta}{\delta\mathcal{V}_i^{\bar\sigma_i\bar\sigma_j}(\tau_i)},\\ D_{\sigma_i\sigma_j}[i,j] &= \sigma_i\sigma_j\frac{\delta}{\delta\mathcal{V}_{i,j}^{\bar\sigma_i\bar\sigma_j}(\tau_i)},\\ \text{and } D[i,i] &= D[i].\end{aligned} \tag{39}$$

In $\gamma[i,i]$ and $\gamma[i]$ we have equal-time objects with creation operators to the left of destruction operators. Let us note the rewriting of the last term in Eq. (26):

$$\begin{aligned}&-\sum_j \mathcal{V}_{ij}^{\sigma_1\sigma_2}(\sigma_i\sigma_1)\langle\langle X_i^{\bar\sigma_1\bar\sigma_i}(\tau_i)X_j^{0\sigma_2}(\tau_j)X_f^{\sigma_f 0}(\tau_f)\rangle\rangle\\ &\quad= +\sum_j \mathcal{V}_{ij}^{\sigma_1\sigma_2}\left(\gamma_{\sigma_i\sigma_1}[i] - D_{\sigma_i\sigma_1}[i]\right)\mathcal{G}_{\sigma_2\sigma_f}[j,f].\end{aligned} \tag{40}$$

With this preparation, using Eq. (34) we rewrite Eq. (26) as

$$\begin{aligned}&\left(\partial_{\tau_i} - \boldsymbol{\mu} + \tfrac{1}{4}J_0\right)\mathcal{G}_{\sigma_i\sigma_f}[i,f]\\ &\quad= -\delta[i,f]\left(\delta_{\sigma_i\sigma_f} - \gamma_{\sigma_i\sigma_f}[i]\right) - \mathcal{V}_i^{\sigma_i\sigma_{\mathbf{j}}}\\ &\qquad\times\mathcal{G}_{\sigma_{\mathbf{j}}\sigma_f}[i,f] - \mathcal{V}_{i,\mathbf{j}}^{\sigma_i\sigma_{\mathbf{j}}}(\tau_i)\quad\mathcal{G}_{\sigma_{\mathbf{j}}\sigma_f}[\mathbf{j},f]\\ &\qquad+\mathcal{V}_{i\mathbf{j}}^{\sigma_1\sigma_2}\left[\gamma_{\sigma_i\sigma_1}(i) - D_{\sigma_i\sigma_1}(i)\right]\mathcal{G}_{\sigma_2\sigma_f}(\mathbf{j},f) + t[i,\mathbf{j}]\\ &\qquad\times\left\{\left(\mathbb{1} - \gamma[i] + D[i] - \tfrac{1}{2}\gamma[\mathbf{j}] + \tfrac{1}{2}D[\mathbf{j}]\right)\cdot\mathcal{G}[\mathbf{j},f]\right\}_{\sigma_i\sigma_f}\\ &\qquad+t[i,\mathbf{j}]\left\{\left(-\tfrac{1}{2}\gamma[\mathbf{j},i] + \tfrac{1}{2}D[\mathbf{j},i]\right)\cdot\mathcal{G}[i,f]\right\}_{\sigma_i\sigma_f}\\ &\qquad+\tfrac{1}{2}J[i,\mathbf{j}]\left\{(\gamma[\mathbf{j}] - D[\mathbf{j}])\cdot\mathcal{G}[i,f]\right\}_{\sigma_i\sigma_f},\end{aligned} \tag{41}$$

where the fixed variables are in normal letters and the repeated variables in bold letters are summed in space and integrated in time. This may be written compactly in matrix form as

$$\begin{aligned}&\left(\partial_{\tau_i} - \boldsymbol{\mu}\right)\mathcal{G}[i,f]\\ &\quad= -\delta[i,f](\mathbb{1} - \gamma[i]) - \mathcal{V}_i\cdot\mathcal{G}[i,f]\\ &\qquad- \mathcal{V}_{i,\mathbf{j}}\cdot\mathcal{G}[\mathbf{j},f] + (\gamma(i) - D[i])\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\mathcal{G}[\mathbf{j},f]\\ &\qquad- X[i,\mathbf{j}]\cdot\mathcal{G}[\mathbf{j},f] - Y[i,\mathbf{j}]\cdot\mathcal{G}[\mathbf{j},f],\end{aligned} \tag{42}$$

where we used the definitions (with fixed j and summed $\mathbf{k}$)

$$\begin{aligned}X[i,j] &= -t[i,j]\left(D[i] + \tfrac{1}{2}D[j]\right)\\ &\qquad+\delta[i,j]\tfrac{1}{2}(J[i,\mathbf{k}]D[\mathbf{k}] - t[i\mathbf{k}]D[\mathbf{k},i]),\\ Y[i,j] &= -t[i,j]\left(\mathbb{1} - \gamma[i] - \tfrac{1}{2}\gamma[j]\right) + \tfrac{1}{4}J_0\mathbb{1}\\ &\qquad-\delta[i,j]\tfrac{1}{2}\left(J[i,\mathbf{k}]\gamma[\mathbf{k}] - t[i,\mathbf{k}]\gamma[\mathbf{k},i]\right).\end{aligned} \tag{43}$$

These exact equations Eq. (42) and Eq. (43) form the basis for the remaining discussion. The coefficients in X and Y differ slightly from the ones in Ref. 2, in view of the usage of the effective Hermitean Hamiltonian idea in this paper. The extra terms arise from the form of Eq. (33), and actually vanish if we could treat either of these exactly. We will show that this formulation leads to approximations obeying the shift theorems I and II discussed earlier; note however that Eq. (42) and the forms of X,Y in Eq. (43) are manifestly invariant under these theorems.

III. DECOMPOSITION OF $\mathcal{G}$ INTO THE AUXILIARY FERMION GREEN'S FUNCTION g AND THE CAPARISON FACTOR μ

As discussed in the introduction, we next write the *product ansatz* for $\mathcal{G}$

$$\mathcal{G}[a,b] = \mathbf{g}[a,\mathbf{r}]\cdot\mu[\mathbf{r},b], \tag{44}$$

where $\mathbf{g}$ is the canonical auxiliary Green's function and μ is the caparison factor, or the adaptive spectral weight. Since $\mathcal{G}$ satisfies antiperiodic boundary conditions under $\tau_a \to \tau_a + \beta$ and $\tau_b \to \tau_b + \beta$ separately, we must Fourier-transform both factors $\mathbf{g}$ and μ with fermionic frequencies $\omega_n = (2n+1)\pi k_B T$. At this point μ and $\mathbf{g}$ are undetermined. Let us first note in matrix notation the equal-time objects:

$$\begin{aligned}\gamma[i] &= \mathcal{G}[i^-,i] \to (\mathbf{g}[i,\mathbf{a}]\cdot\mu[\mathbf{a},i])^{(k)}\\ &= (\mu[\mathbf{a},i])^{(k)}\cdot(\mathbf{g}[i,\mathbf{a}])^{(k)},\\ \gamma[i,j] &= \mathcal{G}[j^-,i] \to (\mathbf{g}[j,\mathbf{a}]\cdot\mu[\mathbf{a},i])^{(k)}\\ &= (\mu[\mathbf{a},i])^{(k)}\cdot(\mathbf{g}[j,\mathbf{a}])^{(k)}.\end{aligned} \tag{45}$$

We define three-point vertex functions

$$\begin{aligned}\Lambda_{\sigma_3\sigma_4}^{\sigma_1\sigma_2}(p,q;r) &\equiv -\frac{\delta}{\delta\mathcal{V}_r^{\sigma_3\sigma_4}(\tau_r)}\left\{\mathbf{g}_{\sigma_1\sigma_2}^{-1}[p,q]\right\},\\ \mathcal{U}_{\sigma_3\sigma_4}^{\sigma_1\sigma_2}[a,b;c] &\equiv \frac{\delta\mu_{\sigma_1\sigma_2}[a,b]}{\delta\mathcal{V}_c^{\sigma_3\sigma_4}(\tau_c)},\end{aligned} \tag{46}$$

or as an implicit matrix in the upper indices (but explicit in the lower ones):

$$\begin{aligned}\Lambda_{\sigma_3\sigma_4}(p,q;r) &= -\frac{\delta}{\delta\mathcal{V}_r^{\sigma_3\sigma_4}}\{\mathbf{g}^{-1}[p,q]\},\\ \mathcal{U}_{\sigma_3\sigma_4}[a,b;c] &\equiv \frac{\delta\mu[a,b]}{\delta\mathcal{V}_c^{\sigma_3\sigma_4}}.\end{aligned} \tag{47}$$

In a similar vein, to obtain the four-point vertex functions corresponding to the source $\mathcal{V}_{rs}$ with a pair of points r,s with $\tau_r = \tau_s$, we define

$$\begin{aligned}\Lambda_*(p,q;r,s) &= -\frac{\delta}{\delta\mathcal{V}_{r,s}^*(\tau_r)}\{\mathbf{g}^{-1}[p,q]\},\\ \mathcal{U}_*[a,b;c,d] &\equiv \frac{\delta\mu[a,b]}{\delta\mathcal{V}_{c,d}^*(\tau_c)}.\end{aligned} \tag{48}$$

In some expressions involving summations, it is convenient to think of the vertices $\Lambda_*(p,q;r,s),\mathcal{U}_*[p,q;r,s]$ with independent times τ_r,τ_s, with the constraint of equal times imposed by multiplying by a delta function $\delta(\tau_r - \tau_s)$, as illustrated in Eq. (B4).

This set of vertices Λ and $\mathcal{U}$ replaces the single vertex Γ of a canonical many-body system, and we will also find equations determining these below. Clearly in any exact treatment, the

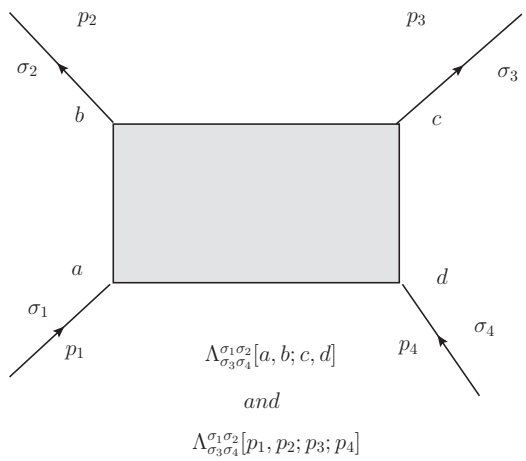


FIG. 3. The four-site vertex can be visualized from its definition for canonical theory: $-\langle\langle f_{a\sigma_1} f^\dagger_{b\sigma_2} f^\dagger_{c\sigma_3} f_{d\sigma_4}\rangle\rangle + \langle\langle f_{a\sigma_1} f^\dagger_{b\sigma_2}\rangle\rangle\langle\langle f^\dagger_{c\sigma_3} f_{d\sigma_4}\rangle\rangle = \frac{\delta}{\delta\mathcal{V}^{\sigma_3\sigma_4}_{cd}}\mathbf{g}_{\sigma_1\sigma_2}(ab) = \mathbf{g}_{\sigma_1\sigma'_1}[a,\mathbf{a}]\Lambda^{\sigma'_1\sigma'_2}_{\sigma_3\sigma_4}[\mathbf{a},\mathbf{b};c,d]\mathbf{g}_{\sigma'_2\sigma_2}[\mathbf{b},b]$. Therefore we may visualize that apart from the external legs, $\Lambda^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[a,b;c,d] \sim \langle f_{a\sigma_1} f^\dagger_{b\sigma_2} f^\dagger_{c\sigma_3} f_{d\sigma_4}\rangle$. Note that in this convention, the labels differ by a cyclic permutation from those in Fig. 2.

four-point vertex contains the three-point vertex by collapsing the points:

$$\Lambda^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}(p,q;r) = \Lambda^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}(p,q;r,s\to r), \tag{49}$$

and similarly for $\mathcal{U}$. However in any approximation scheme, this identity would follow only if the single-occupancy constraint at a given site i, namely $\langle\langle X_i^{\sigma_1\sigma_2} X_i^{0\sigma_3}\ldots\rangle\rangle = 0$, is satisfied exactly, for all choices of the spin indices. Since typical approximations relax this constraint, if only slightly, it is useful to keep both sets of vertices in the theory as separate entities. Another attractive possibility is to require the identity Eq. (49), by making a different set of (controlled) approximations, and is also discussed below. Figure 3 illustrates the conventions used for the four-point vertex; the three-point vertex is obtained by the indicated contraction.

We now use a notation where $*$ is used as a place holder, as illustrated in component form by

$$\cdots\xi^*_{\sigma_a\sigma_b}\cdots\frac{\delta}{\delta\mathcal{V}^*_{\mathbf{j}}} = \cdots\sigma_a\sigma_b\cdots\frac{\delta}{\delta\mathcal{V}^{\bar\sigma_a,\bar\sigma_b}_{\mathbf{j}}}, \tag{50}$$

with $\xi_{\sigma_a\sigma_b} = \sigma_a\sigma_b$, and an implicit spin flip in the indices of the attached derivative operator $\delta/\delta\mathcal{V}^{\bar\sigma_a,\bar\sigma_b}_{\mathbf{j}}$.

We would like to rewrite Eq. (42) in terms of the vertex functions. We need to express

$$\begin{aligned} X[i,\mathbf{j}]\cdot\mathcal{G}[\mathbf{j},f] &= -t[i,\mathbf{j}]\left(D[i]+\tfrac{1}{2}D[\mathbf{j}]\right)\cdot\mathcal{G}[\mathbf{j},f] \\ &\quad+\tfrac{1}{2}\left(J[i,\mathbf{k}]D[\mathbf{k}]-t[i\mathbf{k}]D[\mathbf{k},i]\right)\cdot\mathcal{G}[i,f] \end{aligned} \tag{51}$$

in terms of the vertex functions. Differentiating Eq. (44) we find

$$\begin{aligned} \frac{\delta}{\delta\mathcal{V}^{\sigma,\sigma'}_r}\mathcal{G}[a,b] &= \mathbf{g}[a,\mathbf{c}]\cdot\Lambda_{\sigma,\sigma'}(\mathbf{c},\mathbf{d};r)\cdot\mathcal{G}[\mathbf{d},b] \\ &\quad+\mathbf{g}[a,\mathbf{c}]\cdot\mathcal{U}_{\sigma,\sigma'}[\mathbf{c},b;r]. \end{aligned} \tag{52}$$

Consulting Eq. (39) for the definition of $D_{\sigma_1\sigma_2}[i] = \xi_{\sigma_1\sigma_2}\frac{\delta}{\delta\mathcal{V}_i^{\bar\sigma_1\bar\sigma_2}}$, where $\xi_{\sigma_1\sigma_2} = \sigma_1\sigma_2$, we rewrite this as

$$\begin{aligned} D[r]\cdot\mathcal{G}[a,b] &= \xi^*\cdot\mathbf{g}[a,\mathbf{c}]\cdot\Lambda_*(\mathbf{c},\mathbf{d};r)\cdot\mathcal{G}[\mathbf{d},b] \\ &\quad+\xi^*\cdot\mathbf{g}[a,\mathbf{c}]\cdot\mathcal{U}_*[\mathbf{c},b;r], \end{aligned} \tag{53}$$

where the spin flip in the derivatives is implied as stressed above.

Combining Eq. (51) and Eq. (53) we define the useful linear operator

$$\begin{aligned} \mathbf{L}[i,j] &= t[i,\mathbf{k}]\xi^*\cdot\mathbf{g}[\mathbf{k},j]\cdot\left(\frac{\delta}{\delta\mathcal{V}_i^*}+\frac{1}{2}\frac{\delta}{\delta\mathcal{V}_{\mathbf{k}}^*}\right) \\ &\quad+\frac{1}{2}t[i,\mathbf{k}]\xi^*\cdot\mathbf{g}[i,j]\cdot\frac{\delta}{\delta\mathcal{V}^*_{\mathbf{k},i}} \\ &\quad-\frac{1}{2}J[i,\mathbf{k}]\xi^*\cdot\mathbf{g}[i,j]\cdot\frac{\delta}{\delta\mathcal{V}_{\mathbf{k}}^*}. \end{aligned} \tag{54}$$

Hence we may write Eq. (51) compactly as

$$X[i,\mathbf{j}]\cdot\mathcal{G}[\mathbf{j},f] \equiv \Phi[i,\mathbf{b}]\cdot\mathcal{G}[\mathbf{b},f]+\Psi[i,f], \tag{55}$$

where the two central objects of this theory arise from the action of a common operator Eq. (54) on two seed objects $\mathbf{g}^{-1}$ and μ as follows:

$$\begin{aligned} \Phi[i,m] &\equiv \mathbf{L}[i,\mathbf{c}]\cdot\mathbf{g}^{-1}[\mathbf{c},m] \\ &= -t[i,\mathbf{j}]\xi^*\cdot\mathbf{g}[\mathbf{j},\mathbf{c}]\cdot\left(\Lambda_*[\mathbf{c},m;i]+\tfrac{1}{2}\Lambda_*[\mathbf{c},m;\mathbf{j}]\right) \\ &\quad-\tfrac{1}{2}t[i,\mathbf{k}]\,\xi^*\cdot\mathbf{g}[i,\mathbf{c}]\cdot\Lambda_*[\mathbf{c},m;\mathbf{k},i] \\ &\quad+\tfrac{1}{2}J[i,\mathbf{k}]\,\xi^*\cdot\mathbf{g}[i,\mathbf{c}]\cdot\Lambda_*[\mathbf{c},m;\mathbf{k}] \end{aligned} \tag{56}$$

and

$$\begin{aligned} \Psi[i,m] &\equiv -\mathbf{L}[i,\mathbf{c}]\cdot\mu[\mathbf{c},m] \\ &= -t[i,\mathbf{j}]\xi^*\cdot\mathbf{g}[\mathbf{j},\mathbf{c}]\cdot\left(\mathcal{U}_*[\mathbf{c},m;i]+\tfrac{1}{2}\mathcal{U}_*[\mathbf{c},m;\mathbf{j}]\right) \\ &\quad-\tfrac{1}{2}t[i,\mathbf{k}]\,\xi^*\cdot\mathbf{g}[i,\mathbf{c}]\cdot\mathcal{U}_*[\mathbf{c},m;\mathbf{k},i] \\ &\quad+\tfrac{1}{2}J[i,\mathbf{k}]\,\xi^*\cdot\mathbf{g}[i,\mathbf{c}]\cdot\mathcal{U}_*[\mathbf{c},m;\mathbf{k}]. \end{aligned} \tag{57}$$

We write Eq. (43) as

$$\begin{aligned} Y[i,j] &= -t[i,j]+Y_1[i,j], \\ Y_1[i,j] &= t[i,j]\left(\gamma[i]+\tfrac{1}{2}\gamma[j]\right) \\ &\quad-\delta[i,j]\tfrac{1}{2}\left(J[i,\mathbf{k}]\gamma[\mathbf{k}]-t[i,\mathbf{k}]\gamma[\mathbf{k},i]\right). \end{aligned} \tag{58}$$

We also need to process the object:

$$\begin{aligned} &(\gamma(i)-D[i])\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\mathcal{G}[\mathbf{j},f] \\ &\quad= \gamma(i)\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\mathcal{G}[\mathbf{j},f]-\xi^*\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\frac{\delta}{\delta\mathcal{V}_i^*}\mathcal{G}[\mathbf{j},f] \\ &\quad= \gamma(i)\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\mathcal{G}[\mathbf{j},f]-\xi^*\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\mathbf{g}[\mathbf{j},\mathbf{c}]\cdot\Lambda_*[\mathbf{c},\mathbf{r};i] \\ &\qquad\cdot\mathcal{G}[\mathbf{r},f]-\xi^*\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\mathbf{g}[\mathbf{j},\mathbf{c}]\cdot\mathcal{U}_*[\mathbf{c},f;i]. \end{aligned} \tag{59}$$

IV. ASSEMBLING THE EQUATIONS

Let us rewrite the three relevant equations symbolically:

(1) Eq. (42) for $\mathcal{G}$:

$$\begin{aligned} (\partial_{\tau_i}-\boldsymbol{\mu})\mathcal{G} &= -\delta(\mathbb{1}-\gamma)-\mathcal{V}_i\cdot\mathcal{G}-\mathcal{V}_{i,\mathbf{j}}\cdot\mathcal{G} \\ &\quad+(\gamma-D_i)\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\mathcal{G}-X\cdot\mathcal{G}-Y\cdot\mathcal{G}. \end{aligned} \tag{60}$$

(2) Eq. (59) for the two site source $\mathcal{V}_{ij}$:

$$(\gamma - D_i)\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\mathcal{G} = \gamma(i)\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\mathcal{G}[\mathbf{j},f] - \xi^*\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\mathbf{g}\cdot\Lambda_*\cdot\mathcal{G} - \xi^*\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\mathbf{g}\cdot\mathcal{U}_*. \tag{61}$$

(3) Eq. (55) the product rule:

$$X.\mathcal{G} = \Phi.\mathcal{G} + \Psi. \tag{62}$$

Combining these we rewrite Eq. (60) symbolically as

$$[\partial_{\tau_i} - \boldsymbol{\mu} + Y + \mathcal{V}_i + (\mathbb{1}-\gamma)\cdot\mathcal{V}_{i,\mathbf{j}} + \xi^*\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\mathbf{g}\cdot\Lambda_* + \Phi]\mathcal{G} = -\delta(\mathbb{1}-\gamma) - \Psi - \xi^*\cdot\mathcal{V}_{i,\mathbf{j}}\cdot\mathbf{g}\cdot\mathcal{U}_*. \tag{63}$$

Defining

$$\mathbf{g}_0^{-1}[i,f] = \big\{\big[\big(\boldsymbol{\mu} - \partial_{\tau_i} - \tfrac{1}{4}J_0\big)\mathbb{1} - \mathcal{V}_i\big]\delta[i,f] + t[i,f] - \mathcal{V}_{i,f}(\tau_i)\delta(\tau_i - \tau_f)\big\}, \tag{64}$$

the exact EOM Eq. (42) can be written in matrix form:

$$\big\{\mathbf{g}_0^{-1}[i,\mathbf{j}] + \gamma_i\cdot\mathcal{V}_{i,\mathbf{j}} - \xi^*\cdot\mathcal{V}_{i,\mathbf{a}}\cdot\mathbf{g}[\mathbf{a},\mathbf{b}]\cdot\Lambda_*(\mathbf{b},\mathbf{j};i) - Y_1[i,\mathbf{j}] - \Phi[i,\mathbf{j}]\big\}\cdot\mathbf{g}[\mathbf{j},\mathbf{f}]\cdot\mu[\mathbf{f},f] = \delta[i,f](\mathbb{1}-\gamma[i]) + \Psi[i,f] + \xi^*\cdot\mathcal{V}_{i,\mathbf{a}}\cdot\mathbf{g}[\mathbf{a},\mathbf{b}]\cdot\mathcal{U}_*(\mathbf{b},f;i). \tag{65}$$

At this point, a convenient parameter λ (finally set $\lambda\to 1$) is now inserted into this equation as follows:

$$\big\{\mathbf{g}_0^{-1}[i,\mathbf{j}] + \underbrace{\lambda\gamma_i\cdot\mathcal{V}_{i,\mathbf{j}} - \lambda\xi^*\cdot\mathcal{V}_{i,\mathbf{a}}\cdot\mathbf{g}[\mathbf{a},\mathbf{b}]\cdot\Lambda_*(\mathbf{b},\mathbf{j};i)} - \lambda\, Y_1[i,\mathbf{j}] - \lambda\Phi[i,\mathbf{j}]\big\}\cdot\mathbf{g}[\mathbf{j},\mathbf{f}]\cdot\mu[\mathbf{f},f] = \delta[i,f](\mathbb{1}-\lambda\gamma[i]) + \lambda\,\Psi[i,f] + \underbrace{\lambda\xi^*\cdot\mathcal{V}_{i,\mathbf{a}}\cdot\mathbf{g}[\mathbf{a},\mathbf{b}]\cdot\mathcal{U}_*(\mathbf{b},f;i)}. \tag{66}$$

Clearly this becomes the exact equation Eq. (65) at $\lambda = 1$, and reduces to the Fermi gas Green's function Eq. (64) at $\lambda = 0$. We may now split Eq. (65) exactly into a pair of equations that are fundamental to the theory:

$$\big\{\mathbf{g}_0^{-1}[i,\mathbf{j}] + \lambda\gamma_i\cdot\mathcal{V}_{i,\mathbf{j}} - \lambda\xi^*\cdot\mathcal{V}_{i,\mathbf{a}}\cdot\mathbf{g}[\mathbf{a},\mathbf{b}]\cdot\Lambda_*(\mathbf{b},\mathbf{j};i) - \lambda\, Y_1[i,\mathbf{j}] - \lambda\Phi[i,\mathbf{j}]\big\}\cdot\mathbf{g}[\mathbf{j},f] = \delta[i,f], \tag{67}$$

$$\mu[i,f] = \delta[i,f](\mathbb{1}-\lambda\gamma[i]) + \lambda\,\Psi[i,f] + \lambda\xi^*\cdot\mathcal{V}_{i,\mathbf{a}}\cdot\mathbf{g}[\mathbf{a},\mathbf{b}]\cdot\mathcal{U}_*(\mathbf{b},f;i). \tag{68}$$

We can usefully invert Eq. (67) and write

$$\mathbf{g}^{-1}[i,m] = \big\{\mathbf{g}_0^{-1}[i,m] + \lambda\gamma_i\cdot\mathcal{V}_{i,m} - \lambda\xi^*\cdot\mathcal{V}_{i,\mathbf{a}}\cdot\mathbf{g}[\mathbf{a},\mathbf{b}]\cdot\Lambda_*(\mathbf{b},m;i) - \lambda\, Y_1[i,m] - \lambda\Phi[i,m]\big\}. \tag{69}$$

We see that $\mathbf{g}$ satisfies a canonical equation, with a delta function of weight unity on the right, and μ soaks up the remaining factors on the right-hand side of Eq. (66). This decomposition is not unique; one has the obvious freedom of respectively post-multiplying $\mathbf{g}$ and pre-multiplying μ by a common function and its inverse. However, requiring $\mathbf{g}$ to be canonical fixes the function to be unity. The motivation of introducing λ in the above equations is to establish adiabatic, or more properly parametric, continuity with the Fermi gas.[16] At this stage some remarks are necessary.

(1) At $\lambda = 1$ Eq. (67) and Eq. (68) become exact equations for the EC phase, while it has the virtue that as $\lambda = 0$ it gives a canonical equation for $\mathbf{g}$, with $\mu[i,j] = \mathbb{1}\delta[i,j]$. Procedurally, we can calculate objects to a given order in λ iteratively, and set $\lambda = 1$ at the end of the calculation. We thus establish and maintain continuity with the Fermi gas in the equations of motion.

(2) The process of introducing λ into the EOM is not unique. For example the terms of Eq. (66) in the underbraces cancel at $i = \mathbf{j}$ from the vanishing of Eq. (40). However this cancellation is exact only at $\lambda = 1$, so we will find below that an expansion in λ has the annoying feature of a slight violation of the contraction of indices result Eq. (49). We will show below that this is inconsequential to the orders in λ considered here. With hindsight, a better strategy would be to impose the constraint Eq. (49) to the order of the calculation. This can be achieved if we multiply the terms in underbraces by a sufficiently high power of λ^r, say with $r \geqslant r_0$, and thereby avoid dealing with this problem at low orders $r < r_0$. Below we will analyze the minimal choice $r = 1$, record the issues that crop up, and make suitable approximations later. The impatient may simply ignore the terms with underbraces.

(3) Another type of freedom is available at this stage: If necessary, we could add an arbitrary term that varies smoothly with λ and vanishes at both end points, e.g., $\propto \lambda(1-\lambda)$, to either side of Eq. (67) and Eq. (68). It will turn out that the first-order term $[\mathbf{g}^{-1}]_1$ calculated below does need a simple term of this type to fulfill the Fermi surface sum rule. In general, however, the natural and minimal choice made in Eq. (66), without such a term, seems adequate for higher terms.

(4) We note that the shift theorems I and II are preserved by X,Y above in Eq. (43), and this invariance survives the introduction of λ in Eq. (66). As a result the various objects $\Phi,\Psi,\mathbf{g}^{-1},\mu$ satisfy these theorems individually. This property leads to a powerful consistency check on the approximations to each order in λ.

(5) Note that a λ expansion of $\gamma[i]$ implies that the high-frequency fall-off of $\mathcal{G}\sim\frac{c_0}{i\omega}$ now occurs with a coefficient $c_0 = 1-\lambda\gamma$ that is different from $1-\frac{n}{2}$ at finite orders of λ. While it is tempting to freeze this coefficient at the exact value, it would be inconsistent since we take its derivatives to find Ψ, etc. The departure of this coefficient from the exact value becomes increasingly significant near $n\sim 1$, and provides a criterion for the validity of a given order of approximation.

V. EXPLICIT EQUATIONS AND THE ZERO-SOURCE LIMIT IN FOURIER SPACE

When we turn off the sources, the various matrix function $\mathcal{G},\mathbf{g},\mu$ become spin diagonal. We will also take Fourier transforms (only) in this limit, since translation invariance in space and time is regained when the sources vanish.

We next express Φ and Ψ explicitly in terms of the vertex functions. We need to take the Fourier transform of Eq. (56) and Eq. (57). In the ECFL theory, a rotationally invariant liquid phase is obtained by turning off the sources. We can use the standard spin rotational symmetry analysis illustrated here with Λ as in Ref. 11. We define the three nonvanishing matrix elements as $\Lambda^{(1)} = \Lambda^{\sigma\sigma}_{\sigma\sigma}$, $\Lambda^{(2)} = \Lambda^{\sigma\sigma}_{\bar\sigma\bar\sigma}$, and $\Lambda^{(3)} = \Lambda^{\sigma\bar\sigma}_{\sigma\bar\sigma}$. We also record the Nozières identity for the

two expressions of a particle-hole singlet, $\Lambda^{(1)} - \Lambda^{(2)} = \Lambda^{(3)}$, which provides an important check on the theory. We further use a notation for the frequently occurring antisymmetric combination $\Lambda^{(a)} = \Lambda^{(2)} - \Lambda^{(3)}$. Armed with these, we next drop the matrix structure by utilizing an identity arising with a fixed σ (such as in the expression for $\Phi_{\sigma\sigma}$ above):

$$\begin{aligned}\langle\sigma|\xi^*\cdot\mathbf{g}\cdot\Lambda_*|\sigma\rangle &= \sum_{\sigma_a\sigma_b}\sigma\sigma_a\mathbf{g}_{\sigma_a\sigma_b}\Lambda^{\sigma_b\sigma}_{\bar\sigma\bar\sigma_a}\\ &= \sum_{\sigma_b}\left(\mathbf{g}_{\sigma\sigma_b}\Lambda^{\sigma_b\sigma}_{\bar\sigma\bar\sigma} - \mathbf{g}_{\bar\sigma\sigma_b}\Lambda^{\sigma_b\sigma}_{\bar\sigma\sigma}\right)\\ &= \left(\mathbf{g}_{\sigma\sigma}\Lambda^{\sigma\sigma}_{\bar\sigma\bar\sigma} - \mathbf{g}_{\bar\sigma\bar\sigma}\Lambda^{\bar\sigma\sigma}_{\bar\sigma\sigma}\right)\\ &= \mathbf{g}(\Lambda^{(2)} - \Lambda^{(3)}) \equiv \mathbf{g}\Lambda^{(a)}. \end{aligned} \tag{70}$$

Note that we dropped the spin index on $\mathbf{g}$ due to the isotropy of the state.

We use the FT convention for the two-, three-, and four-site objects illustrated with the examples

$$\begin{aligned}\mathcal{G}[a,b] &= \sum_k e^{ik(a-b)}\mathcal{G}(k),\\ \Lambda^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[a,b;c] &= \sum_{p_1,p_2} e^{ip_1(a-c)+ip_2(c-b)}\Lambda^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}(p_1,p_2),\\ \Lambda^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[a,b;c,d] &= \sum_{p_1+p_4=p_2+p_3} e^{i(p_1a-p_2b-p_3c+p_4d)}\\ &\quad\times\Lambda^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}(p_1,p_2;p_3,p_4).\end{aligned} \tag{71}$$

The identity Eq. (49) in momentum space implies

$$\begin{aligned}\Lambda(p_1,p_2) &= \sum_{p_3,p_4}\Lambda(p_1,p_2;p_3,p_4),\\ \mathcal{U}(p_1,p_2) &= \sum_{p_3,p_4}\mathcal{U}(p_1,p_2;p_3,p_4).\end{aligned} \tag{72}$$

At zero source we get the exact relations between self-energies and vertices by Fourier-transforming Eq. (56) and Eq. (57):

$$\begin{aligned}\Phi(k) &= \sum_p\left(\varepsilon_p + \frac{1}{2}\varepsilon_k + \frac{1}{2}J_{k-p}\right)\mathbf{g}[p]\Lambda^{(a)}(p,k)\\ &\quad+\sum_{pq}\frac{1}{2}\varepsilon_{q+p-k}\mathbf{g}[p]\,\Lambda^{(a)}(p,k;q+p-k,q)\\ &= \sum_{pq}\left(\varepsilon_p + \frac{1}{2}\varepsilon_k + \frac{1}{2}\varepsilon_{q+p-k} + \frac{1}{2}J_{k-p}\right)\mathbf{g}[p]\\ &\quad\times\Lambda^{(a)}(p,k;q+p-k,q),\\ \Psi(k) &= \sum_p\left(\varepsilon_p + \frac{1}{2}\varepsilon_k + \frac{1}{2}J_{k-p}\right)\mathbf{g}[p]\mathcal{U}^{(a)}(p,k)\\ &\quad+\sum_{pq}\frac{1}{2}\varepsilon_{q+p-k}\,\mathbf{g}[p]\mathcal{U}^{(a)}(p,k;q+p-k,q)\\ &= \sum_{pq}\left(\varepsilon_p + \frac{1}{2}\varepsilon_k + \frac{1}{2}\varepsilon_{q+p-k} + \frac{1}{2}J_{k-p}\right)\\ &\quad\times\mathbf{g}[p]\,\mathcal{U}^{(a)}(p,k;q+p-k,q).\end{aligned} \tag{73}$$

A convergence factor $e^{i\omega_p 0^+}$ arises from the time ordering and is implied wherever necessary and the last line in both equations is valid provided the identity Eq. (72) is satisfied. Here $\Lambda^{(a)} = \Lambda^{(2)} - \Lambda^{(3)}$ and $\mathcal{U}^{(a)} = \mathcal{U}^{(2)} - \mathcal{U}^{(3)}$.

With $k = (\vec{k}, i\omega_k)$ and $\omega_n = \pi(2n+1)k_BT$, the Green's functions at a fixed λ read

$$\begin{aligned}\mathcal{G}(k) &= \mathbf{g}(k)\times\mu(k),\\ \mathbf{g}^{-1}[k] &= i\omega_n + \boldsymbol{\mu} - \varepsilon_k - \tfrac{1}{4}J_0 - \lambda Y_1(k) - \lambda\Phi(k),\\ \mu[k] &= 1 - \lambda\gamma + \lambda\Psi(k).\end{aligned} \tag{74}$$

The sum rule for the number of physical particles and the auxiliary fermions is given by

$$\sum_p \mu[p]\mathbf{g}[p] = \frac{n}{2}, \tag{75}$$

$$\sum_p \mathbf{g}[p] = \frac{n}{2}. \tag{76}$$

While the sum rule Eq. (75) clearly counts the number of physical electrons, the origin of the sum rule Eq. (76) for $\mathbf{g}$ requires some discussion taken from Ref. 2. We recall that it is meant to enforce the Luttinger-Ward theorem of a conserved Fermi volume for the auxiliary fermions. By so doing and through the composition $\mathcal{G} = \mathbf{g}\times\mu$, it also preserves it for the physical fermions. While $\boldsymbol{\mu}$ provides us with one obvious Lagrange multiplier to enforce one of the sum rules, the more subtle parameter u_0, introduced in Eq. (27), is required to enforce the second sum rule Eq. (91). Explicit expressions for γ, Y_1, Φ, Ψ can be calculated at various orders in λ as demonstrated below.

TABLE I. Summary of defining equations. The computation of the Green's function $\mathcal{G} = \mathbf{g}\cdot\mu$ in Eq. (44) requires several intermediate variables. The complete set of variables in this theory (first column) and their mutual and λ dependence (second column) are collected here for convenience. The corresponding equation number in the paper is given in the last column.

Object	Defining Equation	Eq. No.
$\mathbf{g}^{-1}[i,m]$	$\{\mathbf{g}_0^{-1}[i,m] + \lambda\gamma_i\cdot\mathcal{V}_{i,m} - \lambda\xi^*\cdot\mathcal{V}_{i,\mathbf{a}}\cdot\mathbf{g}[\mathbf{a},\mathbf{b}]\cdot\Lambda_*(\mathbf{b},m;i) - \lambda\, Y_1[i,m] - \lambda\Phi[i,m]\}$	Eq. (69)
$\mu[i,m]$	$\delta[i,m]\,(\mathbb{1} - \lambda\gamma[i]) + \lambda\,\Psi[i,m] + \lambda\xi^*\cdot\mathcal{V}_{i,\mathbf{a}}\cdot\mathbf{g}[\mathbf{a},\mathbf{b}]\cdot\mathcal{U}_*(\mathbf{b},m;i)$	Eq. (68)
$Y_1[i,m]$	$t[i,m](\gamma[i] + \frac{1}{2}\gamma[m]) - \delta[i,m]\frac{1}{2}\,(J[i,\mathbf{k}]\gamma[\mathbf{k}] - t[i,\mathbf{k}]\gamma[\mathbf{k},i])$	Eq. (58)
$\gamma[i]$	$\mu^{(k)}[\mathbf{a},i]\cdot\mathbf{g}^{(k)}[i,\mathbf{a}]$	Eq. (45)
$\gamma[i,m]$	$\mu^{(k)}[\mathbf{a},i]\cdot\mathbf{g}^{(k)}[m,\mathbf{a}]$	Eq. (45)
$\Phi[i,m]$	$-t[i,\mathbf{j}]\xi^*\cdot\mathbf{g}[\mathbf{j},\mathbf{c}]\cdot\left(\Lambda_*[\mathbf{c},m;i] + \frac{1}{2}\Lambda_*[\mathbf{c},m;\mathbf{j}]\right) - \frac{1}{2}t[i,\mathbf{k}]\,\xi^*\cdot\mathbf{g}[i,\mathbf{c}]\cdot\Lambda_*[\mathbf{c},m;\mathbf{k},i] + \frac{1}{2}J[i,\mathbf{k}]\,\xi^*\cdot\mathbf{g}[i,\mathbf{c}]\cdot\Lambda_*[\mathbf{c},m;\mathbf{k}]$	Eq. (56)
$\Psi[i,m]$	$-t[i,\mathbf{j}]\xi^*\cdot\mathbf{g}[\mathbf{j},\mathbf{c}]\cdot\left(\mathcal{U}_*[\mathbf{c},m;i] + \frac{1}{2}\mathcal{U}_*[\mathbf{c},m;\mathbf{j}]\right) - \frac{1}{2}t[i,\mathbf{k}]\,\xi^*\cdot\mathbf{g}[i,\mathbf{c}]\cdot\mathcal{U}_*[\mathbf{c},m;\mathbf{k},i] + \frac{1}{2}J[i,\mathbf{k}]\,\xi^*\cdot\mathbf{g}[i,\mathbf{c}]\cdot\mathcal{U}_*[\mathbf{c},m;\mathbf{k}]$	Eq. (57)

TABLE II. Vertex functions. The theory requires three-point and four-point vertices. Their nomenclature (first column) and definition (second column) are given, along with the corresponding equation number in the paper.

Vertex	Defining Equation	Eq. No.
$\Lambda^{\sigma_a\sigma_b}_{\sigma_c\sigma_d}[i,m;j]$	$-\frac{\delta}{\delta\mathcal{V}_j^{\sigma_c\sigma_d}}\mathbf{g}^{-1}_{\sigma_a\sigma_b}[i,m]$	Eq. (46)
$\Lambda^{\sigma_a\sigma_b}_{\sigma_c\sigma_d}[i,m;j,k]$	$-\frac{\delta}{\delta\mathcal{V}_{j,k}^{\sigma_c\sigma_d}}\mathbf{g}^{-1}_{\sigma_a\sigma_b}[i,m]$	Eq. (48)
$\mathcal{U}^{\sigma_a\sigma_b}_{\sigma_c\sigma_d}[i,m;j]$	$\frac{\delta}{\delta\mathcal{V}_j^{\sigma_c\sigma_d}}\mu_{\sigma_a\sigma_b}[i,m]$	Eq. (46)
$\mathcal{U}^{\sigma_a\sigma_b}_{\sigma_c\sigma_d}[i,m;j,k]$	$\frac{\delta}{\delta\mathcal{V}_{j,k}^{\sigma_c\sigma_d}}\mu_{\sigma_a\sigma_b}[i,m]$	Eq. (48)

VI. SUMMARIZING

Before proceeding to the iterative scheme, we collect all the relevant equations for convenience in Table I. The various vertex functions are found from relationships summarized in Table II.

It is worthwhile to provide one nontrivial example of the matrix notation. In component form note that $\Phi[i,m]$ can be written out as

$$\begin{aligned}\Phi_{\sigma_i\sigma_m}[i,m] = &-t[i,\mathbf{j}]\sigma_i\sigma_1\mathbf{g}_{\sigma_1\sigma_2}[\mathbf{j},\mathbf{c}]\\ &\times\left(\Lambda^{\sigma_2\sigma_m}_{\bar\sigma_i\bar\sigma_1}[\mathbf{c},m;i]+\tfrac{1}{2}\Lambda^{\sigma_2\sigma_m}_{\bar\sigma_i\bar\sigma_1}[\mathbf{c},m;\mathbf{j}]\right)\\ &-\tfrac{1}{2}t[i,\mathbf{k}]\,\sigma_i\sigma_1\mathbf{g}_{\sigma_1\sigma_2}[i,\mathbf{c}]\Lambda^{\sigma_2\sigma_m}_{\bar\sigma_i\bar\sigma_1}[\mathbf{c},m;\mathbf{k},i]\\ &+\tfrac{1}{2}J[i,\mathbf{k}]\,\sigma_i\sigma_1\mathbf{g}_{\sigma_1\sigma_2}[i,\mathbf{c}]\Lambda^{\sigma_2\sigma_m}_{\bar\sigma_i\bar\sigma_1}[\mathbf{c},m;\mathbf{k}].\end{aligned}$$

VII. λ EXPANSION AND THE ITERATIVE SCHEME

Taking functional derivatives with respect to $\mathcal{V}$, we generate a self-energy–vertex hierarchy of fermionic theory, paralleling the standard (i.e., canonical) theory, but with greater complexity due to the two kinds of vertex functions and self-energies. We describe the λ expansion and the iterative process next. The iterations are analogous to the skeleton diagram expansion in standard many-body theory, where λ plays the role of the interaction constant. Various objects are expanded in terms of λ and $\mathbf{g}$, while $\mathbf{g}$ itself is left intact. Potentially confusing is the treatment of $\mathbf{g}^{-1}$, which *is expanded in* λ *and* $\mathbf{g}$, ignoring its obvious relationship as the inverse of $\mathbf{g}$. This becomes understandable when we recall that $\mathbf{g}^{-1}$ is, apart from $\mathbf{g}_0^{-1}$, the Dyson self-energy of the auxiliary system, and is to be regarded as a functional of $\mathbf{g}$, as in the Luttinger-Ward functional Ref. 17. One example of this expansion may be useful. Consider $\gamma[i,m]$; we will expand it as

$$\begin{aligned}\gamma^{(k)}[i,m] = \mathbf{g}[m,\mathbf{a}]\cdot\mu[\mathbf{a},i] = \mathbf{g}[m,\mathbf{a}]\cdot([\mu[\mathbf{a},i]]_0\\ +\lambda(\mu[\mathbf{a},i]]_1+\lambda^2[\mu[\mathbf{a},i]]_2+O(\lambda^3)),\end{aligned}\tag{77}$$

keeping $\mathbf{g}$ intact, i.e., unexpanded in λ. A similar expansion is carried out also for $\gamma[i]$, leading to a correction of the high-frequency fall of coefficient c_0 as noted above.

Iterative process. We now describe the various steps of the iteration process. First note that all variables (except $\mathbf{g}$) are expanded as

$$\mathcal{A} = [\mathcal{A}]_0+\lambda[\mathcal{A}]_1+\lambda^2[\mathcal{A}]_2+\cdots+\lambda^p[\mathcal{A}]_p+\cdots.\tag{78}$$

The iteration scheme can be summarized in the two following tables. Table III lists the seed objects needed at any order and gives the derived objects. Table IV lists the higher order objects and the needed lower level objects for stepping up.

(I) *Initialization at* $p=0$. The iterations require the following starting relations:

$$\begin{aligned}\mathbf{g}_0^{-1}[i,m] &= \left\{\left[\left(\boldsymbol{\mu}-\partial_{\tau_i}-\tfrac{1}{4}J_0\right)\mathbb{1}-\mathcal{V}_i\right]\right.\\ &\quad\left.\times\,\delta[i,m]+t[i,m]-\mathcal{V}_{i,m}\right\},\\ [\mu[i,f]]_0 &= \mathbb{1}\delta[i,f].\end{aligned}\tag{79}$$

(II) *Computation of derived objects at level p from Table I*. The set of equations requiring $[\mu[i,m]]_p$:

$$\begin{aligned}[\gamma[i]]_p &= [\mu^{(k)}[\mathbf{a},i]]_p\cdot\mathbf{g}^{(k)}[i,\mathbf{a}],\\ [\gamma[i,m]]_p &= [\mu^{(k)}[\mathbf{a},i]]_p\cdot\mathbf{g}^{(k)}[m,\mathbf{a}],\\ \left[\mathcal{U}^{\sigma_a\sigma_b}_{\sigma_c\sigma_d}[i,m;j]\right]_p &= \left(\frac{\delta}{\delta\mathcal{V}_j^{\sigma_c\sigma_d}}\right)\left[\mu_{\sigma_a\sigma_b}[i,m]\right]_p,\\ \left[\mathcal{U}^{\sigma_a\sigma_b}_{\sigma_c\sigma_d}[i,m;j,k]\right]_p &= \left(\frac{\delta}{\delta\mathcal{V}_{j,k}^{\sigma_c\sigma_d}}\right)\left[\mu_{\sigma_a\sigma_b}[i,m]\right]_p,\end{aligned}\tag{80}$$

TABLE IV. Iteration level step-up calculations. In proceeding upwards in the iterative process in Eq. (84) the computed $(p+1)$th-order objects are listed in the first column, and the pth-order objects needed are in the second column. Since $\mathbf{g}^{-1}$ and μ at a given level suffice to determine all other objects at that level through Table III, the iterative nature of the scheme becomes transparent.

Level $(p+1)$ Object	Required Level p Objects
$[\mu[i,m]]_{p+1}$	$[\gamma[i],\ \Psi[i,m],\mathcal{U}[a,b;c],\ \mathcal{U}[a,b;c,d]]_p$
$\left[\mathbf{g}^{-1}[i,m]\right]_{p+1}$	$[Y_1[i,m],\Phi[i,m],\Lambda[a,b;c]]_p$

TABLE III. Iteration level p calculations. The auxiliary inverse Green's function $\mathbf{g}^{-1}$ and the adaptive spectral weight μ play the role of seed objects at the pth order. By computing them to pth order in the parameter λ, we obtain the vertex functions and the other variables listed in the second column to the same order as described in Eqs. (80)–(83).

Seed Object	Derived Objects
$[\mu[i,m]]_p$	$[\gamma[i],\gamma[i,m],Y_1[i,m],\mathcal{U}[a,b;c],\ \mathcal{U}[a,b;c,d]]_p$
$[\mathcal{U}[a,b;c],\mathcal{U}[a,b;c,d]]_p$	$[\Psi[i,m]]_p$
$[\mathbf{g}^{-1}[i,m]]_p$	$[\Lambda[a,b;c],\Lambda[a,b;c,d]]_p$
$[\Lambda[a,b;c],\Lambda[a,b;c,d]]_p$	$[\Phi[i,m]]_p$

$$[Y_1[i,m]]_p = t[i,m]\left[\gamma[i] + \frac{1}{2}\gamma[m]\right]_p - \delta[i,m]\frac{1}{2}\left[J[i,\mathbf{k}]\gamma[\mathbf{k}] - t[i,\mathbf{k}]\gamma[\mathbf{k},i]\right]_p, \quad (81)$$

$$\begin{aligned}[\Psi[i,m]]_p &= -t[i,\mathbf{j}]\xi^*\cdot\mathbf{g}[\mathbf{j},\mathbf{c}]\cdot\left(\mathcal{U}_*[\mathbf{c},m;i] + \frac{1}{2}\mathcal{U}_*[\mathbf{c},m;\mathbf{j}]\right)_p \\ &\quad - \frac{1}{2}t[i,\mathbf{k}]\,\xi^*\cdot\mathbf{g}[i,\mathbf{c}]\cdot(\mathcal{U}_*[\mathbf{c},m;\mathbf{k},i])_p \\ &\quad + \frac{1}{2}J[i,\mathbf{k}]\,\xi^*\cdot\mathbf{g}[i,\mathbf{c}]\cdot(\mathcal{U}_*[\mathbf{c},m;\mathbf{k}])_p\,. \end{aligned} \quad (82)$$

The set of equations requiring $[\mathbf{g}^{-1}[i,m]]_p$:

$$\begin{aligned}\left[\Lambda^{\sigma_a\sigma_b}_{\sigma_c\sigma_d}[i,m;j]\right]_p &= -\left(\frac{\delta}{\delta\mathcal{V}^{\sigma_c\sigma_d}_j}\right)\left[\mathbf{g}^{-1}_{\sigma_a\sigma_b}[i,m]\right]_p, \\ \left[\Lambda^{\sigma_a\sigma_b}_{\sigma_c\sigma_d}[i,m;j,k]\right]_p &= -\left(\frac{\delta}{\delta\mathcal{V}^{\sigma_c\sigma_d}_{j,k}}\right)\left[\mathbf{g}^{-1}_{\sigma_a\sigma_b}[i,m]\right]_p, \\ [\Phi[i,m]]_p &= -t[i,\mathbf{j}]\xi^*\cdot\mathbf{g}[\mathbf{j},\mathbf{c}] \\ &\quad\cdot\left(\Lambda_*[\mathbf{c},m;i] + \frac{1}{2}\Lambda_*[\mathbf{c},m;\mathbf{j}]\right)_p \\ &\quad - \frac{1}{2}t[i,\mathbf{k}]\,\xi^*\cdot\mathbf{g}[i,\mathbf{c}]\cdot(\Lambda_*[\mathbf{c},m;\mathbf{k},i])_p \\ &\quad + \frac{1}{2}J[i,\mathbf{k}]\,\xi^*\cdot\mathbf{g}[i,\mathbf{c}]\cdot(\Lambda_*[\mathbf{c},m;\mathbf{k}])_p\,. \end{aligned} \quad (83)$$

(III) *Level p to level $(p+1)$, step up equations*:

$$\begin{aligned}[\mu[i,m]]_{p+1} &= -\delta[i,m][\gamma[i]]_p + [\Psi[i,m]]_p \\ &\quad + [\xi^*\cdot\mathcal{V}_{i,\mathbf{a}}\cdot\mathbf{g}(\mathbf{a},\mathbf{b})\cdot\mathcal{U}_*(\mathbf{b},m;i)]_p, \\ [\mathbf{g}^{-1}[i,m]]_{p+1} &= [\gamma_i\cdot\mathcal{V}_{i,m} - \xi^*\cdot\mathcal{V}_{i,\mathbf{a}}\cdot\mathbf{g}(\mathbf{a},\mathbf{b})\cdot\Lambda_*(\mathbf{b},m;i)]_p \\ &\quad - [Y_1[i,m] + \Phi[i,m]]_p. \end{aligned} \quad (84)$$

(IV) *If required level is reached, exit; otherwise return to step II.*

This iterative procedure can thus be applied to obtain equations for the Green's functions to any desired order. In practice the higher order terms grow very rapidly, as in the Feynman diagram series. However, as explained in the introduction, a low-order expansion is expected to capture already the significant features of extreme correlations, an important reason being that the range is finite and small; i.e., $\lambda \in [0,1]$. In this work we will be content to work to $O(\lambda^2)$ where all the relevant objects can be calculated explicitly.

Second-order Green's function. Having formulated the iterative process, we next apply this to obtain the second-order Green's functions. The calculations are detailed in Appendix B, and we directly present the first- and second-order results here. Displaying the so far hidden u_0 coefficient, we write the complete set of equations to $O(\lambda^2)$ from Eq. (B51) and Eq. (B48):

$$\begin{aligned}\mathcal{G}[k] &= \mathbf{g}(k)\times\mu[k], \\ \mu[k] &= 1 - \lambda\frac{n}{2} + \lambda^2\frac{n^2}{4} - \lambda^2\sum_{p,q}(\varepsilon_p + \varepsilon_{k+q-p} + \varepsilon_k + \varepsilon_q \\ &\quad + J_{k-p} - u_0)\mathbf{g}[p]\mathbf{g}[q]\mathbf{g}[q+k-p] + O(\lambda^3), \end{aligned} \quad (85)$$

$$\begin{aligned}\mathbf{g}^{-1}[k] &= i\omega_n + \boldsymbol{\mu}' - \left(1 - \lambda n + \lambda^2\frac{3n^2}{8}\right)\varepsilon_k \\ &\quad + \lambda\sum_q\frac{1}{2}J_{k-q}\mathbf{g}[q] - \lambda^2\,[\Phi(k)]_1 + O(\lambda^3), \end{aligned} \quad (86)$$

$$\begin{aligned}[\Phi(k)]_1 &= -\sum_{q,p}\mathbf{g}[q]\mathbf{g}[p]\mathbf{g}[k+q-p] \\ &\quad\times(\varepsilon_k + \varepsilon_p + \varepsilon_q + \varepsilon_{k+q-p} + J_{k-p} - u_0) \\ &\quad\times\left\{\varepsilon_k + \varepsilon_p + \varepsilon_q + \varepsilon_{k+q-p} + \frac{1}{2}(J_{k-p} + J_{p-q}) - u_0\right\}. \end{aligned} \quad (87)$$

The shifted chemical potential $\boldsymbol{\mu}'$ is related to the physical (i.e., thermodynamical) chemical potential $\boldsymbol{\mu}$ and u_0 through

$$\begin{aligned}\boldsymbol{\mu}' &= \boldsymbol{\mu} - u_0\frac{\lambda n}{2}\left(1 - \frac{\lambda n}{4}\right) \\ &\quad + \left[J_0\frac{\lambda n}{4}\left(1 - \frac{\lambda n}{2}\right) + 2\lambda\left(1 - \frac{\lambda n}{8}\right)\sum_q\varepsilon_q\mathbf{g}[q]\right]. \end{aligned} \quad (88)$$

In using this expansion, one must first set $\lambda \to 1$. These expressions satisfy the shift theorem I.1 and shift theorem II, as one can verify by shifting ε_k and J_k by k-independent constants, and using $\sum_q \mathbf{g}[q] = \frac{n}{2}$. The self-energy from a Feynman diagram theory to second-order from H_{eff} in Eq. (27) matches the above expression for $\mathbf{g}^{-1}$. The required diagrams are shown in Fig. 4 up to second order where the zigzag line W_{eff} is defined in Fig. 2.

Apart from a single term (the expansion of Y_1 in λ), the expansion of the auxiliary Fermi liquid is largely "autonomous,"

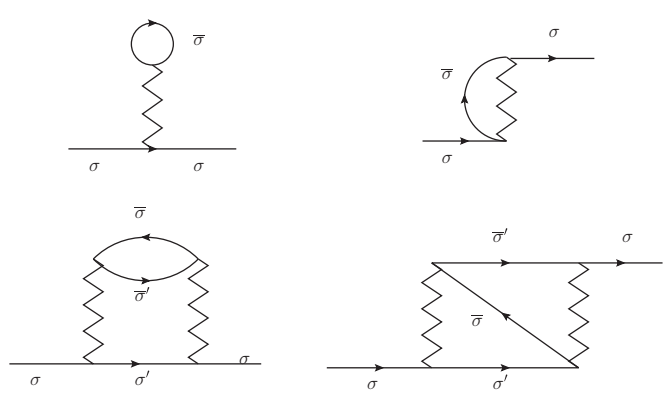


FIG. 4. The self-energy graphs to second order from W_{eff} and the effective Hamiltonian H_{eff}. These determine the Φ self-energy.

i.e., proceeds without requiring the knowledge of μ, and is represented in Feynman diagrammatic terms. The caparison term μ has no obvious interpretation in terms of $H_{\rm eff}$, but is easy to compute along lines similar to the ones shown here, and the full theory splices the two factors to yield $\mathcal{G}$, as described here.

A consistent first-order, i.e., $O(\lambda)$, theory for $\mathbf{g}^{-1}$ and μ can be found after dropping all $O(\lambda^2)$ terms. As it stands, we would get $\mu = 1 - \lambda\frac{n}{2}$ to this order, and this would violate the Fermi surface volume theorem (Ref. 12). To recover from this, we may however set $\mu[k]$ to unity instead. Formally this is achieved by adding $\lambda(1-\lambda)\frac{n}{2}$ to $\mu[k]$ as discussed below Eq. (66), since this added term vanishes at both end points $\lambda = 0$ and $\lambda = 1$. This procedure is within the permissible adjustments of the continuity argument, and at second order cancels out so that the quoted second-order result is unchanged. Further all vertices are unchanged since this is a static term. In this way the first-order theory can also be arranged to satisfy the Luttinger-Ward Fermi volume theorem. This theory has a band dispersion $(1-n)\varepsilon_k$ that shrinks in width by a factor $(1-n)$ as in the Gutzwiller-Brinkman-Rice theory,[7,18] with an enhanced effective mass $m/m^* = (1-n)$. The second-order result presented here provides a more interesting and frequency-dependent correction to the Fermi gas.

In summary, the physical Green's function is obtained from

$$\mathcal{G}[k] = \mathbf{g}[k]\mu[k]. \tag{89}$$

The number of the physical electrons is fixed by the first sum rule,

$$\frac{n}{2} = \sum_k \mathcal{G}[k]e^{i\omega_n 0^+}, \tag{90}$$

while the auxiliary fermion satisfies an identical sum rule,

$$\frac{n}{2} = \sum_k \mathbf{g}[k]e^{i\omega_n 0^+}. \tag{91}$$

We can determine the two independent real parameters $\boldsymbol{\mu}$ and u_0 in order to satisfy both these equations simultaneously, and thus the role of u_0 as a Lagrange multiplier, similar to that of $\boldsymbol{\mu}$, is now evident. It is also clear that the shifts of t or J can be absorbed in the two Lagrange multipliers $\boldsymbol{\mu}$ and u_0. It is worth noting that the simplified ECFL model used in Ref. 2 and Ref. 9 can be obtained from Eq. (85) and Eq. (87) by throwing out the band energies and exchange energies in the coefficients of $\mathbf{g}(q)\mathbf{g}(p)\mathbf{g}(k+q-p)$ while retaining u_0, so that the Lagrange multiplier of that approximation Δ_0 is related to u_0.

The role of the two sum rules in fixing the number of fermions and also the Luttinger-Ward Fermi surface is already discussed in Ref. 2 and above. We can add to that discussion with the help of the explicit functional forms found above. It should be noted from Eq. (85) and Eq. (87) that the functional derivatives

$$I[k,p] \equiv \frac{\delta\,[\Phi[k]]_1}{\delta\mathbf{g}[p]}, \quad J[k,p] \equiv \frac{\delta\,[\Psi[k]]_1}{\delta\mathbf{g}[p]} \tag{92}$$

are symmetric functions under $k \leftrightarrow p$. This symmetry therefore guarantees the existence of two Luttinger-Ward-type functionals of the auxiliary Green's function $\mathbf{g}$,

$$\begin{aligned}\Omega_\Phi[\mathbf{g}] &= -\frac{1}{4}\sum_{k,p,q,r} W(k,q;r,p)[W(k,q;r,p)\\ &\quad + W(k,q;p,r)]\mathbf{g}[k]\mathbf{g}[p]\mathbf{g}[q]\mathbf{g}[r],\\ \Omega_\Psi[\mathbf{g}] &= \frac{1}{4}\sum_{k,p,q,r} W(k,q;r,p)\mathbf{g}[k]\mathbf{g}[p]\mathbf{g}[q]\mathbf{g}[r],\end{aligned} \tag{93}$$

such that the two self-energies can be found from these functionals:

$$[\Phi[k]]_1 = \frac{\delta\Omega_\Phi}{\delta\mathbf{g}[k]}, \quad [\Psi[k]]_1 = \frac{\delta\Omega_\Psi}{\delta\mathbf{g}[k]}. \tag{94}$$

The form of these two functionals follows to this order from Eq. (87), and it is natural to conjecture that such functionals exist to all orders in λ. The existence of the Ω_Φ functional guarantees a (FS) volume-conserving Luttinger-Ward Fermi surface for the $\mathbf{g}$ electrons, and the smooth behavior of $\Psi(k)$ near this surface guarantees likewise for the physical electrons.

VIII. WARD IDENTITIES

This theory admits Ward identities involving the vertices Λ and $\mathcal{U}$ that guarantee current conservation in a similar fashion as Ref. 11. This is displayed with the help of sources, the charge potential $u[m] = \sum_\sigma \mathcal{V}_m^{\sigma\sigma}$ and an added source $v[m]$ coupling to the kinetic energy as

$$t[i,j] \to t[i,j](1 + v[j] - v[i]), \tag{95}$$

so that $v[j] - v[i]$ acts as a discrete version of the Peierls phase factor of electromagnetic coupling in tight binding systems. We define

$$D_m \equiv \partial_{\tau_m}\frac{\delta}{\delta u[m]} - \frac{\delta}{\delta v[m]}, \tag{96}$$

so that the Ward identity expressing the conservation of current, from Ref. 11, reads

$$D_m\mathcal{G}[i,f] = (\delta[i,m] - \delta[f,m])\mathcal{G}[i,f]. \tag{97}$$

This is a discrete (Takahashi type) version of the usual Ward identity appropriate to the lattice Fermi system at hand, and electromagnetic coupling only requires the long-wavelength limit of this identity. We will define the $(\mathcal{T})$ vertices (summing over σ)

$$\begin{aligned}\Lambda^{(\mathcal{T})}(i,j;m) &= -\frac{\delta}{\delta v[m]}\mathbf{g}^{-1}_{\sigma\sigma}[i,j]|_{u,v\to 0},\\ \mathcal{U}^{(\mathcal{T})}(i,j;m) &= \frac{\delta}{\delta v[m]}\mu_{\sigma\sigma}[i,j]|_{u,v\to 0}.\end{aligned} \tag{98}$$

It is easy to see that the bare τ vertices are given by differentiating $\mathbf{g}_0^{-1}$ in Eq. (64) as

$$\begin{aligned}\lambda^{(\mathcal{T})}(i,j;m) &= t[i,j]\,(\delta[i,m] - \delta[j,m])\,,\\ \lambda^{(\mathcal{T})}[p_1,p_2] &= \varepsilon_{p_1} - \varepsilon_{p_2},\end{aligned} \tag{99}$$

while the singlet (i.e., density) vertices are already known from $\Lambda^{(s)} = \sum_{\sigma\sigma'}\Lambda^{\sigma\sigma}_{\sigma'\sigma'}$. Note that the $(\mathcal{T})$ type vertices are antisymmetric in $i \leftrightarrow j$ or $p_1 \leftrightarrow p_2$.

Taking Fourier transforms in Eq. (97) and writing $\mathcal{G} = \mathbf{g} \times \mu$, we get the conservation law:

$$\begin{aligned}&\big(i\omega_{p_1} - i\omega_{p_2}\big)(\mathbf{g}[p_1]\Lambda^{(s)}(p_1,p_2)\mathbf{g}[p_2]\mu[p_2]\\&\quad+\mathbf{g}[p_1]\mathcal{U}^{(s)}(p_1,p_2)) - (\mathbf{g}[p_1]\Lambda^{(\mathcal{T})}(p_1,p_2)\mathbf{g}[p_2]\mu[p_2]\\&\quad+\mathbf{g}[p_1]\mathcal{U}^{(\mathcal{T})}(p_1,p_2)) = \mathbf{g}[p_2]\mu[p_2] - \mathbf{g}[p_1]\mu[p_1].\end{aligned} \tag{100}$$

Canceling out $\mathbf{g}[p_1]\mathbf{g}[p_2]$ we get the Ward identity:

$$\begin{aligned}&\big(i\omega_{p_1} - i\omega_{p_2}\big)(\Lambda^{(s)}(p_1,p_2)\mu[p_2] + \mathcal{U}^{(s)}(p_1,p_2)\mathbf{g}^{-1}[p_2])\\&\quad-(\Lambda^{(\mathcal{T})}(p_1,p_2)\mu[p_2] + \mathcal{U}^{(\mathcal{T})}(p_1,p_2)\mathbf{g}^{-1}[p_2])\\&\quad=\mathbf{g}^{-1}[p_1]\mu[p_2] - \mathbf{g}^{-1}[p_2]\mu[p_1].\end{aligned} \tag{101}$$

With $i\omega_n \to z_n$, we rewrite this as

$$\mathcal{W}_g(p_1,p_2)\mu[p_2] + \mathbf{g}^{-1}[p_2]\mathcal{W}_\mu(p_1,p_2) = 0, \tag{102}$$

where we have defined the two Ward functions:

$$\begin{aligned}\mathcal{W}_g(p_1,p_2) &= (z_1 - z_2)\Lambda^{(s)}(p_1,p_2) - \Lambda^{(\mathcal{T})}(p_1,p_2)\\&\quad+\mathbf{g}^{-1}[p_2] - \mathbf{g}^{-1}[p_1],\\\mathcal{W}_\mu(p_1,p_2) &= (z_1 - z_2)\mathcal{U}^{(s)}(p_1,p_2) - \mathcal{U}^{(\mathcal{T})}(p_1,p_2)\\&\quad+\mu[p_1] - \mu[p_2].\end{aligned} \tag{103}$$

Since p_1 and p_2 are arbitrary, the two terms must vanish separately giving us the pair of Ward identities:

$$\mathcal{W}_g(p_1,p_2) = 0, \tag{104}$$

$$\mathcal{W}_\mu(p_1,p_2) = 0. \tag{105}$$

IX. RANDOM PHASE APPROXIMATION

Since the Green's functions are known to $O(\lambda^2)$, we can take the derivatives of Eq. (B7) and Eq. (B8) to get vertices to this order. Here we calculate by taking the equations to $O(\lambda)$ only, but assuming $\frac{\delta}{\delta\mathcal{V}}\mathbf{g} = \mathbf{g}\Lambda\mathbf{g}$ rather than $\frac{\delta}{\delta\mathcal{V}}\mathbf{g} = \mathbf{g}\mathbf{g}$, thereby obtaining the analog of the RPA. Since the spin susceptibility is also of considerable interest, we will calculate the required vertices in the that channel as well. Summarizing the results we write linear integral equations for the $\mathcal{U}$ vertices:

$$\begin{aligned}\mathcal{U}^{(\mathcal{T})}[p_1,p_2] &= -\lambda\sum_q \mathbf{g}[q]\Lambda^{(\mathcal{T})}(q,q+p_2-p_1)\\&\quad\times\mathbf{g}[q+p_2-p_1] + O(\lambda^2),\\\mathcal{U}^{(s)}[p_1,p_2] &= -\lambda\sum_q \mathbf{g}[q]\Lambda^{(s)}(q,q+p_2-p_1)\\&\quad\times\mathbf{g}[q+p_2-p_1] + O(\lambda^2),\\\mathcal{U}^{(t)}[p_1,p_2] &= \lambda\sum_q \mathbf{g}[q]\Lambda^{(t)}(q,q+p_2-p_1)\\&\quad\times\mathbf{g}[q+p_2-p_1] + O(\lambda^2),\end{aligned} \tag{106}$$

and similarly for the Λ vertices:

$$\begin{aligned}\Lambda^{(\mathcal{T})}[p_1,p_2] &= (\varepsilon_{p_1} - \varepsilon_{p_2})(1 - \underbrace{\lambda n}) - \lambda\sum_q \mathbf{g}[q]\Lambda^{(\mathcal{T})}(q,q+p_2-p_1)\mathbf{g}[q+p_2-p_1]\mathcal{F}(q,p_1,p_2) + O(\lambda^2),\\\Lambda^{(s)}[p_1,p_2] &= 1 - \lambda\sum_q \mathbf{g}[q]\Lambda^{(s)}(q,q+p_2-p_1)\mathbf{g}[q+p_2-p_1]\mathcal{F}(q,p_1,p_2) + O(\lambda^2),\\\Lambda^{(t)}[p_1,p_2] &= 1 + \lambda\sum_q \mathbf{g}[q]\Lambda^{(t)}(q,q+p_2-p_1)\mathbf{g}[q+p_2-p_1]\mathcal{F}(q,p_1,p_2) + O(\lambda^2),\end{aligned} \tag{107}$$

where we use the shorthand $\mathcal{F}(q,p_1,p_2) \equiv \{\varepsilon_{p_1} + \varepsilon_{p_2} + \varepsilon_q + \varepsilon_{q+p_2-p_1} - u_0 + \frac{1}{2}(J_{p_1-p_2} + J_{q-p_1})\}$. The term in underbrace receives an $O(\lambda)$ contribution from differentiating the explicit v dependence of the transformed $t[i,m] \to t[i,m](1 + v[m] - v[i])$ term in Eq. (B7). It is readily shown by examining the kernel of the integral equations that the solution for $\Lambda^{(\mathcal{T})}(p_1,p_2)$ is antisymmetric under exchanging $p_1 \leftrightarrow p_2$, while $\Lambda^{(s)}(p_1,p_2)$ and $\Lambda^{(t)}(p_1,p_2)$ are symmetric.

These vertices are shown to be compatible with Ward identities to $O(\lambda)$ if used with the first-order versions of the Green's functions Eq. (85) and Eq. (86),

$$\begin{aligned}\mathbf{g}[p] &= i\omega_n + \boldsymbol{\mu}' - (1-\lambda n)\varepsilon_k\\&\quad+\frac{\lambda}{2}\sum_q J_{k-q}\mathbf{g}[q] + O(\lambda^2)\end{aligned} \tag{108}$$

$$\text{and}\quad \mu[p] = 1,$$

by substituting in the expressions Eq. (104) and Eq. (105), and showing the self-consistency of this result. The details of this verification parallel the standard proof in QED and are omitted here. Note that μ must be chosen to be unity rather than $1 - \lambda\frac{n}{2}$ as discussed in the second paragraph below Eq. (86), although this choice is irrelevant to the verification of the Ward identity.

X. TWO-PARTICLE RESPONSE

We are interested in the pair correlations of the density $n_a = \sum_\sigma X_a^{\sigma\sigma}$ and the spin density $S_a^z = \frac{1}{2}\sum_{\sigma_1,\sigma_2}\tau^z_{\sigma_1\sigma_2}X_a^{\sigma_1\sigma_2}$, where τ^z is the usual Pauli matrix. These can be obtained from taking the functional derivatives of the Green's function

$$\Upsilon^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[i,j] = \frac{\delta}{\delta\mathcal{V}_j^{\sigma_3\sigma_4}}\mathcal{G}_{\sigma_1\sigma_2}[i^-,i], \tag{109}$$

and can be conveniently found from taking a limit of the three-site object $\Upsilon^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}(p,q;r) = \frac{\delta}{\delta\mathcal{V}_r^{\sigma_3\sigma_4}}\mathcal{G}_{\sigma_1\sigma_2}[p,q]$. With the singlet and triplet objects denoted with a superscript $\alpha = s,t$, we note the following relationships with the standard charge and spin susceptibilities of interest:

$$\begin{aligned}\langle\langle n_a(\tau_a)n_b(\tau_b)\rangle\rangle &= n^2 - 2\Upsilon^{(s)}(a,b),\\\big\langle\big\langle S_a^z(\tau_a)S_b^z(\tau_b)\big\rangle\big\rangle &= -\tfrac{1}{2}\Upsilon^{(t)}(a,b).\end{aligned} \tag{110}$$

Owing to the bosonic nature of the densities, we have the symmetry $\Upsilon^{(\alpha)}(b,a) = \Upsilon^{(\alpha)}(a,b)$ from which the Fourier transform at $Q \equiv (\vec{Q}, i\Omega_q)$ satisfies the relation:

$$\Upsilon^{(\alpha)}(Q) = \Upsilon^{(\alpha)}(-Q). \tag{111}$$

This symmetry can be used as another test of the consistency of any approximation.

The Green's function in Eq. (109) can be decomposed in to $\mathbf{g}$ and μ as before and we find

$$\begin{aligned}\Upsilon^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}(a,b;r) &= \frac{\delta}{\delta \mathcal{V}_r^{\sigma_3\sigma_4}}\left\{\mathbf{g}_{\sigma_1\sigma_a}[a,\mathbf{a}]\mu_{\sigma_a\sigma_2}[\mathbf{a},b]\right\},\\ &= \left\{\mathbf{g}[a,\mathbf{b}]\Lambda_{\sigma_3\sigma_4}(\mathbf{b},\mathbf{s};r)\mathbf{g}[\mathbf{s},\mathbf{a}]\mu[\mathbf{a},q]\right\}_{\sigma_1\sigma_2}\\ &\quad+\left\{\mathbf{g}[a,\mathbf{b}]\mathcal{U}_{\sigma_3\sigma_4}(\mathbf{b},b;r)\right\}_{\sigma_1\sigma_2},\end{aligned} \tag{112}$$

where the vertex and Υ carry upper spin indices that are part of the matrix product. Turning off the sources, we find the expressions for singlet and triplet response

$$\begin{aligned}\Upsilon^{(\alpha)}(a,b;r) &= \mathbf{g}[a,\mathbf{b}]\Lambda^{(\alpha)}(\mathbf{b},\mathbf{s})\mathbf{g}[\mathbf{s},\mathbf{a}]\mu[\mathbf{a},b]\\ &\quad+\mathbf{g}[a,\mathbf{b}]\mathcal{U}^{\alpha}(\mathbf{b},b;r),\\ \Upsilon^{(\alpha)}(p_1,p_2) &= \mathbf{g}[p_1]\Lambda^{(\alpha)}(p_1,p_2)\mathbf{g}[p_2]\mu[p_2]\\ &\quad+\mathbf{g}[p_1]\mathcal{U}^{(\alpha)}(p_1,p_2),\end{aligned} \tag{113}$$

where $\alpha = s,t$. The definitional distinction between left and right derivatives leads to the asymmetry in the above equations making it necessary to test the consistency Eq. (111) term by term.

Using the zero-source limit notation from Ref. 11,

$$\begin{aligned}&Q^{(1)} = Q^{\sigma\sigma}_{\sigma\sigma}, \quad Q^{(2)} = Q^{\sigma\sigma}_{\bar\sigma\bar\sigma}, \quad Q^{(3)} = Q^{\sigma\bar\sigma}_{\sigma\bar\sigma},\\ &Q^{(a)} = Q^{(2)} - Q^{(3)}, \quad Q^{(s)} = Q^{(1)} + Q^{(2)},\\ &Q^{(t)} = Q^{(1)} - Q^{(2)} = Q^{(3)}.\end{aligned} \tag{114}$$

The charge $\alpha = s$ and spin $\alpha = t$ susceptibilities at finite $Q \equiv (\vec{Q}, i\Omega_q)$ are given by setting $p_2 \to p$ and $p_1 \to p+Q$ and summing over p:

$$\begin{aligned}\Upsilon^{(\alpha)}(Q) &\equiv \sum_p \Upsilon^{(\alpha)}(p,p+Q)\\ &= \sum_p [\mathbf{g}[p]\Lambda^{(\alpha)}(p,p+Q)\mathbf{g}[p+Q]\mu[p+Q]\\ &\quad+\mathbf{g}[p]\mathcal{U}^{(\alpha)}(p,p+Q)].\end{aligned} \tag{115}$$

These are exact expression for the susceptibilities, but as usual require a knowledge of the vertices and Green's functions to give practical results. We can now use the RPA vertices calculated in Sec. IX to give the corresponding expressions.

We denote the susceptibility of the auxiliary fermions as

$$\chi^{(\alpha)}_{\Lambda}(Q) \equiv -\sum_q \mathbf{g}[q]\Lambda^{(\alpha)}(q,q+Q)\mathbf{g}[q+Q], \tag{116}$$

and within RPA we note that $\mu[p]$ is independent of p, and from Eq. (106) we denote that the $\mathcal{U}$ vertices are functions of the momentum difference only:

$$\mathcal{U}^{(\alpha)}[p_1,p_2] = \lambda\xi_\alpha\chi^{(\alpha)}_{\Lambda}(p_2-p_1), \tag{117}$$

where ξ_α is 1 for $\alpha =$ singlet and -1 for $\alpha =$ triplet. Therefore we can sum over the p dependence of the second term and rewrite Eq. (115) as

$$(\Upsilon^{(\alpha)}(Q))_{RPA} = -C_\alpha\chi^{(\alpha)}_{\Lambda}(Q), \tag{118}$$

where $C_\alpha = (\mu - \xi_\alpha\lambda\frac{n}{2})$. It seems more appropriate to reset $\mu = (1-\lambda\frac{n}{2})$ from unity at this level, in order to recover the expected high-frequency behavior in the charge as well as spin channel, so that $C_{\text{singlet}} = (1-\lambda n) \to 1-n$ and $C_{\text{triplet}} = 1$. The vertices Λ are to be computed from Eq. (107) and form a consistent set of equations for the two-particle response in the sense of the usual RPA.

The integral equations must be solved numerically. However in order to display some flavor of the results, we pursue this to the lowest order in λ by iteration, where explicit results can be obtained. Let us define a few frequently occurring generalized polarizability functions for convenience. We will now reinstate $J_k \to J_k - u_0$:

$$\begin{aligned}\chi_0(Q) &= -\sum_q \mathbf{g}[q]\mathbf{g}[q+Q],\\ \chi_1(Q) &= -\sum_q \mathbf{g}[q]\mathbf{g}[q+Q]\{\varepsilon_q + \varepsilon_{q+Q}\},\\ \chi_2(Q) &= \frac{1}{2}\sum_{r,p}\mathbf{g}[r]\mathbf{g}[r+Q]\mathbf{g}[p]\mathbf{g}[p+Q]J_{p-r},\\ F(p+Q,p) &= \sum_r \mathbf{g}[r]\mathbf{g}[r+Q]\Big\{\varepsilon_p + \varepsilon_{p+Q} + \varepsilon_r + \varepsilon_{r+Q}\\ &\quad+\frac{1}{2}(J_Q + J_{p-r})\Big\}.\end{aligned} \tag{119}$$

Here $\chi_0(Q)$ is the standard Lindhard function and is positive in the static limit as $\vec{Q} \to 0$, while the other functions are generalizations thereof.

The answers are

$$\begin{aligned}\Upsilon^{(s)}(Q) &= -(1-\lambda n)\chi_0(Q) - \lambda\big[2\chi_0(Q)\chi_1(Q)\\ &\quad-\big(u_0 - \tfrac{1}{2}J_Q\big)\chi_0^2(Q) + \chi_2(Q)\big],\\ \Upsilon^{(t)}(Q) &= -\chi_0(Q) + \lambda\big[2\chi_0(Q)\chi_1(Q)\\ &\quad+\big(\tfrac{1}{2}J_Q - u_0\big)\chi_0^2(Q) + \chi_2(Q)\big].\end{aligned} \tag{120}$$

It is clear that the role of u_0 enhances the spin susceptibility while decreasing the charge susceptibility. To this order we see that the parity test Eq. (111) is satisfied by using the symmetries of the objects in Eq. (119).

Since the Green's function remains infinitely sharp within the RPA, its usefulness is limited, especially in view of the large frequency-dependent corrections with characteristic asymmetry seen in second-order results in Refs. 2, 9, and 10. A second-order version of RPA seems most desirable, although even without vertex corrections to second order, the single-particle spectral results are very interesting already. It also seems interesting to study phenomenologically the analog of the "bubble" diagram for purposes of extracting the optical conductivity; a scheme that reflects the width of the physical Green's function and satisfies the parity requirement Eq. (111) is given by

$$[\mathcal{U}(Q)]_{\text{phen}} = -\frac{1}{1-n/2}\sum_q \mathcal{G}[q]\mathcal{G}[q+Q], \tag{121}$$

although this expression is not the result a systematic expansion of Eq. (115).

XI. DISCUSSION AND CONCLUSIONS

We have described above a controlled technique of dealing with the t-J model. This extremely correlated Fermi liquid theory is a strong-coupling approach, specifically designed to deal with a hard many-body problem. The considerations begin with the strong-coupling limit of the Hubbard model, leading to the t-J model with a hard constraint of eliminated double occupancy. The Schwinger method gives us a crucial initial platform to deal with this problem. The ensuing exact functional differential equations are made tractable by the introduction of the exact *product ansatz*, $\mathcal{G} = \mathbf{g} \times \mu$, with $\mathbf{g}$ a canonical Green's function of auxiliary electrons and μ the caparison factor. The latter, in turn, is understood as an adaptive spectral weight balancing the requirements at the high- and low-frequency ends of the spectrum. Both objects are expanded in powers of a parameter λ that plays the role of fractional double occupancy. Thus $\lambda = 1$ corresponds to complete elimination of double occupancy whereas $\lambda < 1$ has some residual double occupancy. We thus replace the hard constraint of complete elimination of double occupancy by a softer one or partial removal. In order to provide a natural description of the canonical electrons, we introduce the effective Hamiltonian $H_{\rm eff}$, depending parametrically on λ. In order to obey the shift theorems I and II, we find it obligatory to (re)introduce a Hubbard-type u_0 parameter in this model. It also plays the role of a second chemical potential as explained above. The set of steps followed, in our starting as well as ending up with a Hubbard-type interaction, has a slightly circular feel to it. This recipe is perhaps best understood as a renormalization group type procedure, where the constraint of single occupancy is enforced incrementally and the density of doubly occupied sites is thinned out smoothly. The infinite starting value of U in the t-J model is pushed downward to u_0, typically a fraction of the bandwidth from our numerical studies, albeit in a more general model $H_{\rm eff}$, and is therefore amenable to a perturbative expansion. The form of the $H_{\rm eff}$ and the important role of the shift symmetries in validating the approximations is noteworthy. The hopping t_{ij} is elevated to an interaction constant of the model; this unfamiliar step is kept under check by requiring the two important shift invariances. The Schwinger equation Eq. (42) for $\mathcal{G}$, being an exact statement of the problem, provides us with a rigorous backdrop to the entire procedure. Further our procedure has the advantage of being systematically improvable through the iterative scheme developed here.

We can explore superconductivity at a qualitative level by studying the pairing instabilities of the auxiliary fermions given by $H_{\rm eff}$ via its BCS gap function $\Delta(k)$. In this first approximation, the physical electron order parameter $\langle X_k^{\uparrow 0} X_{-k}^{\downarrow 0}\rangle$ is proportional to that of the auxiliary electrons $\langle f_\uparrow^\dagger(k) f_\downarrow^\dagger(-k)\rangle$, together with the single-occupancy constraint of vanishing upon summing over the wave vector k. Within a generalized Hartree Fock theory, retaining the self-energy correction to first order [as in Eq. (108)] as well as the pairing field average,

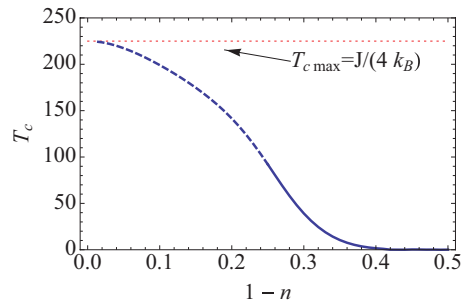


FIG. 5. (Color online) The transition temperature in kelvins, from solving Eq. (122) assuming $t = 3000$ K and $J = 900$ K. The solid line indicates the likely regime of validity of the $O(\lambda)$ theory. Its dotted extension to lower hole density is speculative and is most likely to change with higher order corrections reflecting the nearby Mott insulating state. The dotted red line indicates the maximum T_c obtainable from this scheme, and is seen to depend solely upon the magnitude of J.

we obtain an equation for the gap function $\Delta(k)$:

$$\Delta(k) = \frac{1}{N_s}\sum_p \left\{\varepsilon_k + \varepsilon_p - u_0 + \frac{1}{2}J_{k-p}\right\} \times \Delta(p)\frac{\tanh \beta E(p)/2}{E(p)}, \tag{122}$$

where $E(p) = \sqrt{\Delta^2(p) + \xi_p^2}$, and $\xi_p = \varepsilon_p(1-n) - \frac{1}{2}\sum J_{q-p} n_q - \boldsymbol{\mu}$. In the computation below, we will neglect the numerically small J term in the single-particle energy. Other than u_0 and the two single-particle energies in Eq. (122) required for satisfying the shift theorems I and II, this is the same equation as the one found within the resonating valence bond theory in Refs. 4, 19, and 20. The transition temperature for a d-wave state with a gap function $\Delta(k) = \Delta_d[\cos(k_x) - \cos(k_y)]$ is obtained by solving Eq. (122) for the case of the nearest-neighbor square lattice t-J model, with parameters indicated in the caption of Fig. 5.

It is straightforward to see that the T_c equation has a maximum scale of order $J/(4k_B)$ as already noted in Ref. 19 and Ref. 20. This value is attained in this solution at a higher particle density, or equivalently, a lower hole density, than is warranted by the first approximation. The solid line represents a plausible regime of validity of this scheme.

The extended s-wave order is usually described by a gap function $\Delta(k) = \Delta_{s,0} + \Delta_{s,1}\ [\cos(k_x) + \cos(k_y)]$. The constant term $\Delta_{s,0}$ leads to a finite probability of double occupancy, since it survives a wave vector sum. After it is dropped as per the above discussion, the assumed (purely extended) s-wave order is supported by the J term in the kernel of Eq. (122), but not by the u_0-dependent and single-particle energy terms. The latter thus do not play a role in determining T_c for either d-wave or s-wave orders despite their large magnitude relative to J.

A detailed calculation of the gap equation is planned for the pairing of physical particles, parallel to the $O(\lambda^2)$ theory of the normal state. The finite-lifetime effects are then expected to become relevant. Such an improvement of the pairing scheme should yield a greater understanding of the balance between

the different orders and a greater range of validity in density than the schematic theory treated here.

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APPENDIX A: ATOMIC LIMIT $t = J = 0$

1. Double-occupancy interpretation of λ from the atomic limit

In order to understand the role of λ we study the atomic limit $t, J \to 0$ where this parameter can be introduced into the physical Green's function in the form

$$\mathcal{G}[\lambda, i\omega_n] = \frac{1 - \lambda\frac{n}{2}}{i\omega_n + \boldsymbol{\mu}}, \tag{A1}$$

and study its dependence on λ in the interval [0,1]. The chemical potential $\boldsymbol{\mu}$ can be calculated from the sum rule on the density n of the number of particles N with $n = N/N_s$ and temperature T as

$$\boldsymbol{\mu} = k_B T \ln\left(\frac{n}{2 - (1+\lambda)n}\right). \tag{A2}$$

Thermodynamics tells us that the entropy S can be expressed as

$$S(n) = -N_s \int_0^n dn' \, \frac{\partial \mu(n')}{\partial T}, \tag{A3}$$

and since we know μ from Eq. (A2) we obtain with $y = (1+\lambda)n$

$$\frac{S(n,\lambda)}{k_B N_s} = \frac{1}{1+\lambda}\{\ln 4 - y \ln n - (2-y)\ln(2-y)\}. \tag{A4}$$

We see that its λ derivative $\frac{1}{k_B N_s}\frac{\partial S}{\partial \lambda} = \frac{2}{(1+\lambda)^2}[\frac{y}{2} + \ln(1 - \frac{y}{2})]$ is negative definite. Thus we see that the entropy at a fixed density interpolates monotonically between the free Fermi limit and the infinite U limits as λ ranges over its domain $0 \leqslant \lambda \leqslant 1$. The maximum allowed density is reduced from 2 to $\frac{2}{1+\lambda}$ and thus at $\lambda = 1$ we have a maximum of one electron per site, as expected physically. Thus increasing λ from zero effectively removes the available states contributing to entropy; its role may be viewed as that of (continuous) removal of states. Thus for the equations of motion it is somewhat analogous to the role of Gutzwiller's parameter g in his projection operator $\prod_i [1 - (1-g)n_{i\uparrow}n_{j\downarrow}]$ at the wave function level.

In the atomic limit we can also calculate the entropy at a fixed density of doubly occupied sites $d = \frac{1}{N_s}\sum_i n_{i\uparrow}n_{i\downarrow}$ as

$$\frac{S(n,d)}{k_B N_s} = -d\ln d - (n-2d)\ln\left(\frac{n}{2} - d\right) - (1+d-n)\ln(1+d-n). \tag{A5}$$

An uncorrelated system corresponds to $d = \frac{n^2}{4}$, where the entropy Eq. (A5) is a maximum, while $d = 0$ for the fully projected t-J model. Comparing the two expressions for entropy Eq. (A4) and Eq. (A5), we can express λ in terms of d at any density. We have thus demonstrated that λ is a conjugate variable to the double-occupation density in this limit. Their explicit relationship is illustrated in Fig. 6.

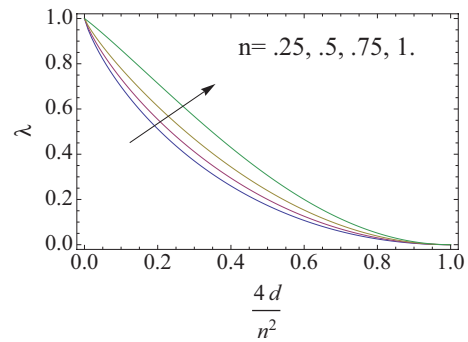

FIG. 6. (Color online) The parameter λ is determined in terms of the double occupancy d at various densities in the atomic limit as described in the text. The arrow indicates increasing density n. Note that the parameter d is scaled into the unit interval.

2. Expansion in λ in the atomic limit

In the atomic limit we set $t \to 0$ and $J \to 0$ so that Eq. (67) and Eq. (68) become

$$\begin{aligned} \mathbf{g}[i,f] &= \mathbf{g}_0[i,f;\boldsymbol{\mu}_a], \\ \mu[i,f] &= \delta[i,f](\mathbb{1} - \lambda\gamma[i]) - \lambda\boldsymbol{\mu}_b\mathbf{g}[i,\mathbf{f}]\cdot\mu[\mathbf{f},f]. \end{aligned} \tag{A6}$$

Here we split the chemical potential into two pieces $\boldsymbol{\mu} = \boldsymbol{\mu}_a + \lambda\boldsymbol{\mu}_b$. Thus in this limit $\mathbf{g}$ is the free Fermi Green's function independent of λ, and $\boldsymbol{\mu}_a$ is the free value $\boldsymbol{\mu}_a \to \boldsymbol{\mu}_0$, the latter determined from the noninteracting theory in terms of the number of particles. If we turn off the source $\mathcal{V}$ the Fourier transforms can be taken as

$$\begin{aligned} \mathbf{g}[i\omega_n] &= \mathbf{g}_0[i\omega_n;\boldsymbol{\mu}_a] = \frac{1}{i\omega_n + \boldsymbol{\mu}_0}, \\ \mu[i\omega_n] &= \left(1 - \lambda\frac{n}{2}\right) - \lambda\boldsymbol{\mu}_b\mathbf{g}[i\omega_n]\mu[i\omega_n], \\ &= \frac{1 - \lambda\frac{n}{2}}{1 + \lambda\boldsymbol{\mu}_b\mathbf{g}[i\omega_n]}. \end{aligned} \tag{A7}$$

Thus the physical Green's function

$$\mathcal{G}[i\omega_n] = \frac{1 - \lambda\frac{n}{2}}{i\omega_n + \boldsymbol{\mu}_0 + \lambda\boldsymbol{\mu}_b}. \tag{A8}$$

We fix the chemical potentials from the number sum rule as usual and thus

$$\begin{aligned} \frac{n}{2} &= \frac{1}{1 + e^{-\beta\boldsymbol{\mu}_0}}, \\ \frac{n}{2} &= \left(1 - \lambda\frac{n}{2}\right)\frac{1}{1 + e^{-\beta(\boldsymbol{\mu}_0 + \lambda\boldsymbol{\mu}_b)}}. \end{aligned} \tag{A9}$$

We may then solve for $\boldsymbol{\mu}$'s in terms of the density and obtain

$$\begin{aligned} \boldsymbol{\mu}_0 &= k_B T \ln\left(\frac{n}{2-n}\right), \\ \lambda\boldsymbol{\mu}_b &= k_B T \ln\left(\frac{2-n}{2-(1+\lambda)n}\right). \end{aligned} \tag{A10}$$

Thus the chemical potential $\boldsymbol{\mu}_1$ has a power series representation

$$\boldsymbol{\mu}_b = \sum_{m=0}^{\infty} \lambda^m \boldsymbol{\mu}_b^{(m)} = k_B T \sum_{m=0}^{\infty} \frac{\lambda^m}{m+1} \left[\frac{n}{2-n}\right]^{m+1}. \tag{A11}$$

We see explicitly from Eq. (A11) that the λ expansion of the the atomic limit is an expansion in $\lambda n/(2-n)$, i.e., a density expansion as well.

APPENDIX B: THE LOW-ORDER CALCULATIONS OF GREEN'S FUNCTIONS

1. Green's function to $O(\lambda)$

We evaluate the complete starting point of the hierarchy. We start with terms of $O(\lambda^0)$ and end with $[\mu]_1$ and $[\mathbf{g}^{-1}]_1$, which are the seeds for the $O(\lambda)$ terms.

a. Seed terms and initialization

$$\begin{aligned} \mathbf{g}_0^{-1}[i,m] &= \big\{\big[\big(\boldsymbol{\mu} - \partial_{\tau_i} - \tfrac{1}{4}J_0\big)\mathbb{1} - \mathcal{V}_i\big] \\ &\quad \times \delta[i,m] + t[i,m] - \mathcal{V}_{i,m}\big\}, \\ [\mu[i,f]]_0 &= \mathbb{1}\delta[i,f]. \end{aligned} \tag{B1}$$

Derived objects:

$$\begin{aligned} [\gamma[i]]_0 &= \mathbf{g}^{(k)}[i,i], \\ [\gamma[i,m]]_0 &= \mathbf{g}^{(k)}[m,i], \\ \big[\mathcal{U}_{\sigma_c\sigma_d}^{\sigma_a\sigma_b}[i,m;j]\big]_0 &= 0, \\ \big[\mathcal{U}_{\sigma_c\sigma_d}^{\sigma_a\sigma_b}[i,m;j,k]\big]_0 &= 0. \end{aligned} \tag{B2}$$

$$\begin{aligned} [Y_1[i,m]]_0 &= t[i,m]\big(\mathbf{g}^{(k)}[i,i] + \tfrac{1}{2}\mathbf{g}^{(k)}[m,m]\big) \\ &\quad - \delta[i,m]\tfrac{1}{2}(J[i,\mathbf{j}]\mathbf{g}^{(k)}[\mathbf{j},\mathbf{j}] - t[i,\mathbf{j}]\mathbf{g}^{(k)}[i,\mathbf{j}]), \\ [\Psi[i,m]]_0 &= 0. \end{aligned} \tag{B3}$$

$$\begin{aligned} \big[\Lambda_{\sigma_c\sigma_d}^{\sigma_a\sigma_b}[i,m;j]\big]_0 &= \delta_{\sigma_a\sigma_c}\delta_{\sigma_b,\sigma_d}\delta[i,j]\delta[j,m], \\ \big[\Lambda_{\sigma_c\sigma_d}^{\sigma_a\sigma_b}[i,m;j,k]\big]_0 &= \delta_{\sigma_a\sigma_c}\delta_{\sigma_b,\sigma_d}\delta[i,j]\delta[m,k]\delta(\tau_j - \tau_k). \end{aligned} \tag{B4}$$

In the four-point vertex above, we have introduced the delta function $\delta(\tau_j - \tau_k)$, so that the labels i,m,j,k can be viewed as four independent space-time variables.

Thus

$$\begin{aligned} [\Phi[i,m]]_0 &= \delta[i,m]t[i,\mathbf{j}]\mathbf{g}^{(k)}[\mathbf{j},i] + \tfrac{1}{2}t[i,m]\mathbf{g}^{(k)}[m,m] \\ &\quad + \tfrac{1}{2}\delta[i,m]t[i,\mathbf{j}]\,\mathbf{g}^{(k)}[i,\mathbf{j}] - \tfrac{1}{2}J[i,m]\mathbf{g}^{(k)}[i,m]. \end{aligned} \tag{B5}$$

Combining the two we get

$$\begin{aligned} &[Y_1[i,m]]_0 + [\Phi[i,m]]_0 \\ &\quad = \delta[i,m]t[i,\mathbf{j}](\mathbf{g}^{(k)}[i,\mathbf{j}] + \mathbf{g}^{(k)}[\mathbf{j},i]) \\ &\qquad + t[i,m](\mathbf{g}^{(k)}[i,i] + \mathbf{g}^{(k)}[m,m]) - \tfrac{1}{2}J[i,m]\mathbf{g}^{(k)}[i,m] \\ &\qquad - \delta[i,m]\tfrac{1}{2}J[i,\mathbf{j}]\mathbf{g}^{(\mathbf{k})}[\mathbf{j},\mathbf{j}]. \end{aligned} \tag{B6}$$

b. Stepping up and final Green's function to $O(\lambda)$

To first order in λ we collect the above results to obtain the Green's function

$$\begin{aligned} [\mathbf{g}^{-1}[i,m]]_1 &= \mathbf{g}^{(k)}[i,i]\cdot\mathcal{V}_{i,m} + \delta[i,m]\mathbf{g}^{(k)}[\mathbf{a},i]\cdot\mathcal{V}_{i,\mathbf{a}}^{(k)} \\ &\quad + \delta[i,m]\tfrac{1}{2}J[i,\mathbf{j}]\mathbf{g}^{(k)}[\mathbf{j},\mathbf{j}] + \tfrac{1}{2}J[i,m]\mathbf{g}^{(k)}[i,m] \\ &\quad - t[i,m](\mathbf{g}^{(k)}[i,i] + \mathbf{g}^{(k)}[m,m]) \\ &\quad - \delta[i,m]t[i,\mathbf{j}](\mathbf{g}^{(k)}[i,\mathbf{j}] + \mathbf{g}^{(k)}[\mathbf{j},i]) \end{aligned} \tag{B7}$$

and the caparison factor

$$[\mu[i,m]]_1 = -\mathbf{g}^{(k)}[i^-,i]\delta[i,m]. \tag{B8}$$

The FTs of these on turning off the sources are found using $\mathbf{g}[i^-,i] \to \frac{n}{2}$ as

$$\begin{aligned} [\mathbf{g}^{-1}[k]]_1 &= n\varepsilon_k - \frac{n}{2}u_0 + \frac{1}{2}\sum_q J_{k-q}\mathbf{g}[q] \\ &\quad + \left(\frac{1}{4}J_0 n + 2\sum_q \varepsilon_q \mathbf{g}[q]\right), \end{aligned} \tag{B9}$$

$$[\mu[k]]_1 = -\frac{n}{2}. \tag{B10}$$

The term $-\frac{n}{2}u_0$ in Eq. (B9) arises when we reinstate $J[i,j] \to J[i,j] - u_0\delta[i,j]$ in Eq. (B7). Let us note that under the shift Eq. (13), the first-order correction $[\mathbf{g}^{-1}[k]]_1$ shifts by $2nu_t + \frac{n}{2}u_J$. Therefore this term is invariant under the shift theorem II and also the shift theorem I.1, provided u_0 is simultaneously transformed as specified in Eq. (31).

2. Green's function to $O(\lambda^2)$

a. μ derived objects

We next start with seed terms of $O(\lambda)$ calculated above and end with $[\mu]_2$ and $[\mathbf{g}^{-1}]_2$:

$$[\mu[i,m]]_1 = -\mathbf{g}^{(k)}[i^-,i]\delta[i,m]. \tag{B11}$$

Let us calculate the derived quantities from the above at the same level:

$$\begin{aligned} [\gamma[i]]_1 &= [\mu^{(k)}[\mathbf{a},i]]_1\cdot\mathbf{g}^{(k)}[i,\mathbf{a}] = -\mathbf{g}[i,i]\cdot\mathbf{g}^{(k)}[i,i], \\ [\gamma[i,m]]_1 &= [\mu^{(k)}[\mathbf{a},i]]_1\cdot\mathbf{g}^{(k)}[m,\mathbf{a}] = -\mathbf{g}[i,i]\cdot\mathbf{g}^{(k)}[m,i], \\ [Y[i,m]]_1 &= -t[i,m]\big(\mathbf{g}[i,i]\cdot\mathbf{g}^{(k)}[i,i] + \tfrac{1}{2}\mathbf{g}[m,m]\cdot\mathbf{g}^{(k)}[m,m]\big) \\ &\quad + \tfrac{1}{2}\delta[i,m]\big(J[i,\mathbf{j}]\mathbf{g}[\mathbf{j},\mathbf{j}]\cdot\mathbf{g}^{(k)}[\mathbf{j},\mathbf{j}] \\ &\quad - t[i,\mathbf{j}]\mathbf{g}[\mathbf{j},\mathbf{j}]\cdot\mathbf{g}^{(k)}[i,\mathbf{j}]\big). \end{aligned} \tag{B12}$$

Zero-source Fourier transforms:

$$\begin{aligned} ([\gamma[0]]_1)_{\mathcal{V}\to 0} &= -\frac{n^2}{4}, \\ ([\gamma[k]]_1)_{\mathcal{V}\to 0} &= -\frac{n}{2}\mathbf{g}[-k], \\ ([Y_1[k]]_1)_{\mathcal{V}\to 0} &= \frac{3n^2}{8}\varepsilon_k - \frac{n^2}{8}u_0 + \left(\frac{n^2}{8}J_0 + \frac{n}{4}\sum_q \varepsilon_q \mathbf{g}[q]\right). \end{aligned} \tag{B13}$$

Here we reinstated $J[i,j] \to J[i,j] - u_0\delta[i,j]$ in Eq. (B12) to obtain the $-\frac{n^2}{8}u_0$ term in Eq. (B13).

b. μ derived vertices

Next we calculate (using lowest-order functional derivatives)

$$\begin{aligned}\left[\mathcal{U}^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[i,m;a]\right]_1 &= -\delta[i,m]\sigma_1\sigma_2\mathbf{g}_{\bar{\sigma}_2\sigma_3}[i,a]\mathbf{g}_{\sigma_4\bar{\sigma}_1}[a,i],\\ \left[\mathcal{U}^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[i,m;a]\right]_{1\ \mathcal{V}\to 0} &= -\delta[i,m]\sigma_1\sigma_2\delta_{\bar{\sigma}_2,\sigma_3}\delta_{\bar{\sigma}_4,\sigma_1}\mathbf{g}[i,a]\mathbf{g}[a,i].\end{aligned} \tag{B14}$$

At zero sources so with $\mathcal{V}\to 0$

$$\begin{aligned}[\mathcal{U}(a)[i,m;a]]_1 &= -2\delta[i,m]\ \mathbf{g}[i,a]\mathbf{g}[a,i],\\ [\mathcal{U}^{(s)}[i,m;a]]_1 &= -\delta[i,m]\ \mathbf{g}[i,a]\mathbf{g}[a,i].\end{aligned} \tag{B15}$$

The zero-source Fourier transforms are as follows:

$$\begin{aligned}\left[\mathcal{U}^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[p_1,p_2]\right]_1 &= -\sigma_1\sigma_2\delta_{\bar{\sigma}_2,\sigma_3}\delta_{\bar{\sigma}_4,\sigma_1}\sum_q \mathbf{g}[q]\mathbf{g}[q+p_2-p_1],\\ \left[\mathcal{U}^{(a)}[p_1,p_2]\right]_1 &= -2\sum_q \mathbf{g}[q]\mathbf{g}[q+p_2-p_1].\end{aligned} \tag{B16}$$

Similarly we find for the four-index vertices

$$\begin{aligned}&\left[\mathcal{U}^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[i,m;a,b]\right]_1\\ &\quad= -\delta[i,m]\ \sigma_1\sigma_2\delta_{\bar{\sigma}_2,\sigma_3}\delta_{\bar{\sigma}_4,\sigma_1}\ \mathbf{g}[i,a]\mathbf{g}[b,i]\ \delta(\tau_a-\tau_b),\\ &[\mathcal{U}^{(a)}[i,m;a,b]]_{1\ \mathcal{V}\to 0}\\ &\quad= -2\delta[i,m]\mathbf{g}[i,a]\mathbf{g}[b,i]\delta(\tau_a-\tau_b).\end{aligned} \tag{B17}$$

The zero-source Fourier transforms are as follows:

$$\begin{aligned}\left[\mathcal{U}^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[p_1,p_2;p_3,p_4]\right]_1 &= -\ \sigma_1\sigma_2\delta_{\bar{\sigma}_2,\sigma_3}\delta_{\bar{\sigma}_4,\sigma_1}\delta_{p_1+p_4,p_2+p_3}\\ &\quad\times\mathbf{g}[p_3]\mathbf{g}[p_4],\\ [\mathcal{U}^{(a)}[p_1,p_2;p_3,p_4]]_1 &= -2\delta_{p_1+p_4,p_2+p_3}\mathbf{g}[p_3]\mathbf{g}[p_4].\end{aligned} \tag{B18}$$

c. Ψ to $O(\lambda)$

We compute $[\Psi]_1$ from these:

$$\begin{aligned}[\Psi(k)]_1 &= \sum_p\left(\varepsilon_p+\frac{1}{2}\varepsilon_k+\frac{1}{2}J_{k-p}\right)\mathbf{g}[p][\mathcal{U}^{(a)}(p,k)]_1\\ &\quad+\sum_{pq}\frac{1}{2}\varepsilon_{q+p-k}\ \mathbf{g}[p][\mathcal{U}^{(a)}(p,k;q+p-k,q)]_1\\ &= -\sum_{p,q}(\varepsilon_p+\varepsilon_{k+q-p}+\varepsilon_k+\varepsilon_q+J_{k-p})\\ &\quad\times\mathbf{g}[p]\mathbf{g}[q]\mathbf{g}[q+k-p]\\ &= \sum_{p,q}W(k,q;q+k-p,p)\mathbf{g}[p]\mathbf{g}[q]\mathbf{g}[q+k-p].\end{aligned} \tag{B19}$$

d. Stepping up: μ to $O(\lambda^2)$

Stepping up, we calculate

$$[\mu[i,m]]_2 = -\delta[i,m]\mathbf{g}[i^-,i]\mathbf{g}^{(k)}[i^-,i]+[\Psi[i,m]]_1. \tag{B20}$$

Hence at zero sources, the Fourier transform reads

$$\begin{aligned}[\mu[k]]_2 &= \frac{n^2}{4}-\sum_{p,q}(\varepsilon_p+\varepsilon_{k+q-p}+\varepsilon_k+\varepsilon_q+J_{k-p})\\ &\quad\times\mathbf{g}[p]\mathbf{g}[q]\mathbf{g}[q+k-p].\end{aligned} \tag{B21}$$

Note that $[\mu]_2$, $[\Psi]_1$ are invariant under all three shift theorems. It is clear that this is a more nontrivial application of the theorems than those in the lowest order.

e. $\mathbf{g}^{-1}$ derived objects

Let us now start with $[\mathbf{g}^{-1}[i,m]]_1$ given in Eq. (B7):

$$\begin{aligned}[\mathbf{g}^{-1}[i,m]]_1 &= \left[\mathbf{g}^{(k)}[i,i]\cdot\mathcal{V}_{i,m}+\delta[i,m]\mathbf{g}^{(k)}[\mathbf{a},i]\cdot\mathcal{V}^{(k)}_{i,\mathbf{a}}\right]\\ &\quad+\left[\delta[i,m]\tfrac{1}{2}J[i,\mathbf{j}]\mathbf{g}^{(k)}[\mathbf{j},\mathbf{j}]+\tfrac{1}{2}J[i,m]\mathbf{g}^{(k)}[i,m]\right]\\ &\quad\times[-t[i,m](\mathbf{g}^{(k)}[i,i]+\mathbf{g}^{(k)}[m,m])\\ &\quad-\delta[i,m]t[i,\mathbf{j}](\mathbf{g}^{(k)}[i,\mathbf{j}]+\mathbf{g}^{(k)}[\mathbf{j},i])].\end{aligned} \tag{B22}$$

f. Vertex functions to $O(\lambda)$

Three-point vertex:

$$\begin{aligned}\left[\Lambda^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[i,m;a]\right]_1 &= -\left(\frac{\delta}{\delta\mathcal{V}^{\sigma_3\sigma_4}_a}\right)\left[\mathbf{g}^{-1}_{\sigma_1\sigma_2}[i,m]\right]_1\\ &= [(I)+(II)+(III)]^{\sigma_1\sigma_2}_{\sigma_3\sigma_4},\end{aligned} \tag{B23}$$

where the terms (I),(II),(III) refer to the three square bracketed terms in Eq. (B22). For the first term we calculate

$$\begin{aligned}(I)^{\sigma_1\sigma_2}_{\sigma_3\sigma_4} &= -\left(\frac{\delta}{\delta\mathcal{V}^{\sigma_3\sigma_4}_a}\right)\left[(\sigma_1\sigma_a)\mathbf{g}_{\bar{\sigma}_a\bar{\sigma}_1}[i,i]\mathcal{V}^{\sigma_a\sigma_2}_{i,m}\right.\\ &\quad\left.+\delta[i,m]\ (\sigma_1\sigma_2)\mathbf{g}_{\bar{\sigma}_a\bar{\sigma}_1}[\mathbf{a},i]\mathcal{V}^{\bar{\sigma}_2\bar{\sigma}_a}_{i,\mathbf{a}}\right],\end{aligned} \tag{B24}$$

$$_{\mathcal{V}\to 0} = 0. \tag{B25}$$

For all other terms we can use a simple calculation:

$$\begin{aligned}\mathcal{X}^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[p,q;r] &= \left(\frac{\delta}{\delta\mathcal{V}^{\sigma_3\sigma_4}_r}\right)\mathbf{g}^{(k)}_{\sigma_1\sigma_2}[p,q]\\ &= (\sigma_1\sigma_2)\mathbf{g}_{\bar{\sigma}_2\sigma_3}[p,r]\mathbf{g}_{\sigma_4\bar{\sigma}_1}[r,q],\\ \mathcal{X}^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[p,q;r]_{\mathcal{V}\to 0} &= (\sigma_1\sigma_2)\delta_{\bar{\sigma}_2\sigma_3}\delta_{\bar{\sigma}_1\sigma_4}\mathbf{g}[p,r]\mathbf{g}[r,q],\\ \mathcal{X}^{(a)}[p,q;r]_{\mathcal{V}\to 0} &= 2\mathbf{g}[p,r]\mathbf{g}[r,q].\end{aligned} \tag{B26}$$

Therefore

$$\begin{aligned}(II)^{(a)}[i,m;a] &= -\delta[i,m]J[i,\mathbf{j}]\mathbf{g}[\mathbf{j},a]\mathbf{g}[a,\mathbf{j}]\\ &\quad-J[i,m]\mathbf{g}[i,a]\mathbf{g}[a,m]\end{aligned} \tag{B27}$$

and

$$\begin{aligned}&(III)^{(a)}[i,m;a]\\ &\quad= 2[t[i,m](\mathbf{g}[i,a]\mathbf{g}[a,i]+\mathbf{g}[m,a]\mathbf{g}[a,m])\\ &\qquad+\delta[i,m]t[i,\mathbf{j}](\mathbf{g}[i,a]\mathbf{g}[a,\mathbf{j}]+\mathbf{g}[\mathbf{j},a]\mathbf{g}[a,i])].\end{aligned} \tag{B28}$$

Zero-source Fourier transforms read as

$$\begin{aligned}(II)^{(a)}[p_1,p_2] &= -J_{p_2-p_1}\sum_q \mathbf{g}[q]\mathbf{g}[q+p_2-p_1] - \sum_q J_{p_1-q}\mathbf{g}[q]\mathbf{g}[q+p_2-p_1],\\ (III)^{(a)}[p_1,p_2] &= -2\sum_q \mathbf{g}[q]\mathbf{g}[q+p_2-p_1]\{\varepsilon_{p_2}+\varepsilon_{p_1}+\varepsilon_{q+p_2-p_1}+\varepsilon_q\}.\end{aligned} \tag{B29}$$

Hence adding up we obtain

$$\begin{aligned}\left[\Lambda^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[p_1,p_2]\right]_1 &= -(\sigma_1\sigma_2)\delta_{\bar\sigma_2\sigma_3}\delta_{\bar\sigma_1\sigma_4}\sum_{p_3,p_4}\delta_{p_1+p_4,p_2+p_3}\mathbf{g}[p_3]\mathbf{g}[p_4]\left\{\varepsilon_{p_1}+\varepsilon_{p_2}+\varepsilon_{p_3}+\varepsilon_{p_4}+\frac{1}{2}\left(J_{p_1-p_2}+J_{p_1-p_3}\right)\right\}\\ &= \frac{1}{2}(\sigma_1\sigma_2)\delta_{\bar\sigma_2\sigma_3}\delta_{\bar\sigma_1\sigma_4}\sum_{p_3,p_4}\mathbf{g}[p_3]\mathbf{g}[p_4]\left[W(p_2,p_3,p_4,p_1)+W(p_2,p_3,p_1,p_4)\right],\end{aligned} \tag{B30}$$

$$[\Lambda^{(a)}[p_1,p_2]]_1 = -\sum_{p_3,p_4}\mathbf{g}[p_3]\mathbf{g}[p_4][W(p_2,p_3,p_4,p_1)+W(p_2,p_3,p_1,p_4)]. \tag{B31}$$

Note that rotation invariance relations imply that since $[\Lambda^{(1)}[p_1,p_2]]_1 = 0$, we must have

$$[\Lambda^{(s)}[p_1,p_2]]_1 = -[\Lambda^{(t)}[p_1,p_2]]_1 = \frac{1}{2}[\Lambda^{(a)}[p_1,p_2]]_1. \tag{B32}$$

Four point vertex. The calculation proceeds similarly:

$$\left[\Lambda^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[i,m;a,b]\right]_1 = -\left(\frac{\delta}{\delta\mathcal{V}^{\sigma_3\sigma_4}_{a,b}}\right)\left[\mathbf{g}^{-1}_{\sigma_1\sigma_2}[i,m]\right]_1 = [(IV)+(V)+(VI)]^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}. \tag{B33}$$

Here the terms (IV)–(VI) refer to the three square bracketed terms in Eq. (B22). For the first term we calculate with implicit $\tau_a = \tau_b$:

$$\begin{aligned}(IV)^{\sigma_1\sigma_2}_{\sigma_3\sigma_4} &= -\left(\frac{\delta}{\delta\mathcal{V}^{\sigma_3\sigma_4}_{a,b}}\right)\left[(\sigma_1\sigma_a)\mathbf{g}_{\bar\sigma_a\bar\sigma_1}[i,i]\mathcal{V}^{\sigma_a\sigma_2}_{i,m}+\delta[i,m]\,(\sigma_1\sigma_2)\mathbf{g}_{\bar\sigma_a\bar\sigma_1}[\mathbf{a},i]\mathcal{V}^{\bar\sigma_2\bar\sigma_a}_{i,\mathbf{a}}\right]\\ &= -\delta[i,a]\delta[m,b]\left[(\sigma_1\sigma_3)\delta_{\sigma_2\sigma_4}\mathbf{g}_{\bar\sigma_3\bar\sigma_1}[i,i]\right]-\delta[i,a]\delta[i,m]\left[(\sigma_1\sigma_2)\delta_{\bar\sigma_2,\sigma_3}\mathbf{g}_{\sigma_4\bar\sigma_1}[b,i]\right],\end{aligned} \tag{B34}$$

$$\begin{aligned}(IV)^{\sigma_1\sigma_2}_{\sigma_3\sigma_4} &\overset{\mathcal{V}\to 0}{} -\delta[i,a]\delta[m,b]\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\mathbf{g}[i,i]-\delta[i,a]\delta[i,m](\sigma_1\sigma_2)\delta_{\sigma_1\bar\sigma_4}\delta_{\sigma_2\bar\sigma_3}\mathbf{g}[b,i],\\ (IV)^{(a)} &= \underbrace{\delta[i,a]\delta[m,b]\mathbf{g}[i,i]-2\delta[i,a]\delta[i,m]\mathbf{g}[b,i]}.\end{aligned} \tag{B35}$$

This term is seen result in a violation of Eq. (49) and Eq. (72) for reasons discussed there and in the second remark below Eq. (68), and therefore is dropped below. We have carried it in the calculation, and demarcated it with the underbrace, in order to see its (minor) contribution explicitly before dropping it.

For all other terms we can use a simple calculation:

$$\begin{aligned}\mathcal{Y}^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[p,q;r,s] &= \left(\frac{\delta}{\delta\mathcal{V}^{\sigma_3\sigma_4}_{r,s}}\right)\mathbf{g}^{(k)}_{\sigma_1\sigma_2}[p,q],\\ \mathcal{Y}^{(a)}[p,q;r,s]_{\mathcal{V}\to 0} &= 2\mathbf{g}[p,r]\mathbf{g}[s,q]\delta(\tau_r-\tau_s).\end{aligned} \tag{B36}$$

Therefore with implicit $\tau_a = \tau_b$:

$$(V)^{(a)}[i,m;a,b] = -\delta[i,m]J[i,\mathbf{j}]\mathbf{g}[\mathbf{j},a]\mathbf{g}[b,\mathbf{j}]-J[i,m]\mathbf{g}[i,a]\mathbf{g}[b,m], \tag{B37}$$

$$\begin{aligned}(VI)^{(a)}[i,m;a,b] &= 2\left[t[i,m](\mathbf{g}[i,a]\mathbf{g}[b,i]+\mathbf{g}[m,a]\mathbf{g}[b,m])+\delta[i,m]t[i,\mathbf{j}]\left(\mathbf{g}[i,a]\mathbf{g}[b,\mathbf{j}]+\mathbf{g}[\mathbf{j},a]\mathbf{g}[b,i]\right)\right],\\ (IV)^{(a)}[i,m;a,b] &= \delta[i,a]\delta[m,b]\mathbf{g}[i,i]-2\delta[i,a]\delta[i,m]\mathbf{g}[b,i],\\ (IV)^{(a)}[p_1,p_2,p_3,p_4] &= \underbrace{\delta_{p_1,p_3}\delta_{p_2,p_4}\mathbf{g}[0^-]-2\delta_{p_1+p_4,p_2+p_3}\mathbf{g}[p_4]},\end{aligned} \tag{B38}$$

$$\begin{aligned}(V)^{(a)}[i,m;a,b] &= -\delta[i,m]J[i,\mathbf{j}]\mathbf{g}[\mathbf{j},a]\mathbf{g}[b,\mathbf{j}]-J[i,m]\mathbf{g}[i,a]\mathbf{g}[b,m],\\ (V)^{(a)}[p_1,p_2,p_3,p_4] &= -\left(J_{p_2-p_1}+J_{p_1-p_3}\right)\mathbf{g}[p_3]\mathbf{g}[p_4]\delta_{p_1+p_4,p_2+p_3},\end{aligned} \tag{B39}$$

$$\begin{aligned}(VI)^{(a)}[i,m;a,b] &= 2\left[t[i,m](\mathbf{g}[i,a]\mathbf{g}[b,i]+\mathbf{g}[m,a]\mathbf{g}[b,m])+\delta[i,m]t[i,\mathbf{j}]\left(\mathbf{g}[i,a]\mathbf{g}[b,\mathbf{j}]+\mathbf{g}[\mathbf{j},a]\mathbf{g}[b,i]\right)\right],\\ (VI)^{(a)}[p_1,p_2,p_3,p_4] &= -2\{\varepsilon_{p_2}+\varepsilon_{p_1}+\varepsilon_{p_3}+\varepsilon_{p_4}\}\mathbf{g}[p_3]\mathbf{g}[p_4]\delta_{p_1+p_4,p_2+p_3}.\end{aligned} \tag{B40}$$

Hence

$$\left[\Lambda^{\sigma_1\sigma_2}_{\sigma_3\sigma_4}[p_1,p_2,p_3,p_4]\right]_1 = -(\sigma_1\sigma_2)\delta_{\bar{\sigma}_2\sigma_3}\delta_{\bar{\sigma}_1\sigma_4}\delta_{p_1+p_4,p_2+p_3}\mathbf{g}[p_3]\mathbf{g}[p_4]\left\{\varepsilon_{p_1}+\varepsilon_{p_2}+\varepsilon_{p_3}+\varepsilon_{p_4}+\tfrac{1}{2}\left(J_{p_1-p_2}+J_{p_1-p_3}\right)\right\}$$
$$\underbrace{-\delta_{p_1,p_3}\delta_{p_2,p_4}\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\mathbf{g}[0^-]-2(\sigma_1\sigma_2)\delta_{\sigma_1\bar{\sigma}_4}\delta_{\sigma_2\bar{\sigma}_3}\delta_{p_1+p_4,p_2+p_3}\mathbf{g}[p_4]}. \tag{B41}$$

Thus

$$[\Lambda^{(a)}[p_1,p_2,p_3,p_4]]_1 = -2\delta_{p_1+p_4,p_2+p_3}\mathbf{g}[p_3]\mathbf{g}[p_4]\left\{\varepsilon_{p_1}+\varepsilon_{p_2}+\varepsilon_{p_3}+\varepsilon_{p_4}+\tfrac{1}{2}\left(J_{p_1-p_2}+J_{p_1-p_3}\right)\right\}$$
$$+\underbrace{\delta_{p_1,p_3}\delta_{p_2,p_4}\mathbf{g}[0^-]-2\delta_{p_1+p_4,p_2+p_3}\mathbf{g}[p_4]}. \tag{B42}$$

Comparing Eq. (B30) and Eq. (B42), we see that other than the term with underbraces, these vertices satisfy Eq. (49) or Eq. (72).

g. Φ to $O(\lambda)$

We now assemble terms:

$$[\Phi(k)]_1 = \sum_p\left(\varepsilon_p+\frac{1}{2}\varepsilon_k+\frac{1}{2}J_{k-p}\right)\mathbf{g}[p][\Lambda^{(a)}(p,k)]_1+\sum_{pq}\frac{1}{2}\varepsilon_{q+p-k}\mathbf{g}[p][\Lambda^{(a)}(p,k;q+p-k,q)]_1. \tag{B43}$$

Let us rewrite this as ($k\to p_2, p\to p_1, q\to p_4$)

$$\begin{aligned}[\Phi(p_2)]_1 &= \sum_{p_1}\left(\varepsilon_{p_1}+\frac{1}{2}\varepsilon_{p_2}+\frac{1}{2}J_{p_1-p_2}\right)\mathbf{g}[p_1][\Lambda^{(a)}(p_1,p_2)]_1+\sum_{p_1+p_4=p_2+p_3}\frac{1}{2}\varepsilon_{p_3}\mathbf{g}[p_1][\Lambda^{(a)}(p_1,p_2;p_3,p_4)]_1\\
&= \underbrace{\frac{n}{4}\sum_{p_3}\varepsilon_{p_3}\mathbf{g}[p_3]-\sum_{p_1,p_4}\varepsilon_{p_1+p_4-p_2}\mathbf{g}[p_1]\mathbf{g}[p_4]}\\
&\quad -2\sum_{p_1+p_4=p_2+p_3}\mathbf{g}[p_1]\mathbf{g}[p_3]\mathbf{g}[p_4]\left(\varepsilon_{p_1}+\frac{1}{2}\varepsilon_{p_2}+\frac{1}{2}J_{p_1-p_2}\right)\left\{\varepsilon_{p_1}+\varepsilon_{p_2}+\varepsilon_{p_3}+\varepsilon_{p_4}+\frac{1}{2}\left(J_{p_1-p_2}+J_{p_1-p_3}\right)\right\}\\
&\quad -\sum_{p_1+p_4=p_2+p_3}\mathbf{g}[p_1]\mathbf{g}[p_3]\mathbf{g}[p_4]\varepsilon_{p_3}\left\{\varepsilon_{p_1}+\varepsilon_{p_2}+\varepsilon_{p_3}+\varepsilon_{p_4}+\frac{1}{2}\left(J_{p_1-p_2}+J_{p_1-p_3}\right)\right\}.\end{aligned} \tag{B44}$$

The first line with underbraces arises from the term Λ in Eq. (B39), or Eq. (B35) and Eq. (B42) which disobey the relation Eq. (49) or Eq. (72). It gives a static but momentum-dependent contribution, and we will drop it as discussed below Eq. (49) and in the second remark below Eq. (68). The rest are combined and rearranged to give

$$\begin{aligned}[\Phi(p_2)]_1 &= -\sum_{p_1+p_4=p_2+p_3}\mathbf{g}[p_1]\mathbf{g}[p_3]\mathbf{g}[p_4]\left(\varepsilon_{p_1}+\varepsilon_{p_2}+\varepsilon_{p_3}+\varepsilon_{p_4}+J_{p_1-p_2}\right)\left\{\varepsilon_{p_1}+\varepsilon_{p_2}+\varepsilon_{p_3}+\varepsilon_{p_4}+\frac{1}{2}\left(J_{p_1-p_2}+J_{p_1-p_3}\right)\right\}\\
&= \frac{1}{2}\sum_{p_1,p_3,p_4}\mathbf{g}[p_1]\mathbf{g}[p_3]\mathbf{g}[p_4]W(p_2,p_3;p_4,p_1)\left[W(p_2,p_3;p_4,p_1)+W(p_2,p_3;p_1,p_4)\right],\end{aligned} \tag{B45}$$

where in the first line we symmetrized further in $p_1\leftrightarrow p_4$.

We can bring this into standard notation by sending $p_2\to k, p_1\to p, p_3\to q, p_4\to k+q-p$:

$$\begin{aligned}[\Phi(k)]_1 &= -\sum_{q,p}\mathbf{g}[q]\mathbf{g}[p]\mathbf{g}[k+q-p](\varepsilon_k+\varepsilon_p+\varepsilon_q+\varepsilon_{k+q-p}+J_{k-p})\left\{\varepsilon_k+\varepsilon_p+\varepsilon_q+\varepsilon_{k+q-p}+\frac{1}{2}(J_{k-p}+J_{p-q})\right\},\\
[\Phi(k)]_1 &= \frac{1}{2}\sum_{q,p}\mathbf{g}[q]\mathbf{g}[p]\mathbf{g}[k+q-p]W(k,q;q+k-p,p)\left[W(k,q;q+k-p,p)+W(k,q;p,q+k-p)\right].\end{aligned} \tag{B46}$$

h. Stepping up and final Green's function to $O(\lambda^2)$

We are now in a position to put together the second-order result for $\mathbf{g}^{-1}$ and also μ. Recall that $[\mathbf{g}^{-1}[k]]_2 = -[Y_1[k]+\Phi[k]]_1$, where these variables are calculated in Eq. (B13) and Eq. (B46). Hence we can now compile the equations of the second-order theory with sources turned off:

$$\begin{aligned}&\mathbf{g}^{-1}(k) = \mathbf{g}_0^{-1}(k)+\lambda[\mathbf{g}^{-1}(k)]_1+\lambda^2[\mathbf{g}^{-1}(k)]_2+O(\lambda^3),\quad [\mathbf{g}^{-1}[k]]_0 = i\omega_n+\boldsymbol{\mu}-\varepsilon_k-\frac{1}{4}J_0,\\
&[\mathbf{g}^{-1}[k]]_1 = n\varepsilon_k-\frac{n}{2}u_0+\frac{1}{2}\sum_q J_{k-q}\mathbf{g}[q]+\left(\frac{1}{4}J_0n+2\sum_q\varepsilon_q\mathbf{g}[q]\right),\\
&[\mathbf{g}^{-1}[k]]_2 = -\frac{3n^2}{8}\varepsilon_k+\frac{n^2}{8}u_0-[\Phi(k)]_1-\left(\frac{n^2}{8}J_0+\frac{n}{4}\sum_q\varepsilon_q\mathbf{g}[q]\right).\end{aligned} \tag{B47}$$

We thus see that all the computed $[\mathbf{g}^{-1}]_j$ are invariant under the two shift theorems. Adding up terms to $O(\lambda^2)$,

$$\mathbf{g}^{-1}[k] = i\omega_n + \boldsymbol{\mu}' - \left(1 - \lambda n + \lambda^2 \frac{3n^2}{8}\right)\varepsilon_k + \lambda \sum_q \frac{1}{2} J_{k-q}\mathbf{g}[q] - \lambda^2 [\Phi(k)]_1 + O(\lambda^3), \tag{B48}$$

$$\boldsymbol{\mu}' = \boldsymbol{\mu} - u_0 \frac{\lambda n}{2}\left(1 - \frac{\lambda n}{4}\right) + \left[J_0 \frac{\lambda n}{4}\left(1 - \frac{\lambda n}{2}\right) + 2\lambda\left(1 - \frac{\lambda n}{8}\right)\sum_q \varepsilon_q \mathbf{g}[q]\right], \tag{B49}$$

with $[\Phi(k)]_1$ defined in Eq. (B46) and a shifted chemical potential $\boldsymbol{\mu}'$. Note that both terms in square brackets in Eq. (B49) are independent of frequency and wave vector; the first (T independent) term may be safely ignored since it vanishes when we finally set $J_0 \to 0$, while the second term involving $\sum_q \varepsilon_q \mathbf{g}[q]$ is expected to be weakly T dependent.

Similarly the caparison factor μ is found to $O(\lambda^2)$ as

$$\mu[k] = 1 + \lambda [\mu[k]]_1 + \lambda^2 [\mu[k]]_2 + O(\lambda^3),$$

$$[\mu[k]]_1 = -\frac{n}{2}, \quad [\mu[k]]_2 = \frac{n^2}{4} + [\Psi[k]]_1 . \tag{B50}$$

Adding up terms to $O(\lambda^2)$ we obtain

$$\mu[k] = 1 - \lambda \frac{n}{2} + \lambda^2 \frac{n^2}{4} + \lambda^2 [\Psi(k)]_1 + O(\lambda^3), \tag{B51}$$

along with the definition in Eq. (B19).

[1] D. Hansen and B. S. Shastry, arXiv:1211.0594 [cond-mat.str-el].

[2] B. S. Shastry, Phys. Rev. Lett. **107**, 056403 (2011); **108**, 029702 (2012).

[3] B. Edegger, V. N. Muthukumar, and C. Gros, Adv. Phys. **56**, 927 (2007).

[4] P. W. Anderson, Science **235**, 1196 (1987).

[5] A. B. Harris and R. V. Lange, Phys. Rev. **157**, 295 (1967).

[6] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).

[7] M. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963).

[8] B. S. Shastry, Phys. Rev. B **84**, 165112 (2011).

[9] G.-H. Gweon, B. S. Shastry, and G. D. Gu, Phys. Rev. Lett. **107**, 056404 (2011).

[10] B. S. Shastry, Phys. Rev. Lett. **109**, 067004 (2012).

[11] B. S. Shastry, Phys. Rev. B **81**, 045121 (2010).

[12] A simple example $\mathcal{G} \sim c_0/(i\omega_n + \mu - \varepsilon_k)$ can be worked out in detail and illustrates this remark.

[13] A. A. Abrikosov, L. Gorkov, and I. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, NJ, 1963).

[14] G. D. Mahan, *Many-Particle Physics*, 3rd ed. (Kluwer-Plenum, 2000).

[15] The magnitude of the relative coefficient 4 in the condition for cancellation $u_J = -4u_t$ is also consistent with a second procedure. In the latter, the shift of t_{ij} and J_{ij} is carried out *after taking the commutator of* $X_i^{0\sigma}$ *with* H, e.g., in the expression Eq. (34), and the extra term in A_{i,σ_i} generated by this process is required to be zero. In general these two procedures can produce different coefficients, as in the minimal theory where one does not symmetrize the expressions. In such cases the coefficient is determined by the one appearing in the equation after taking the commutator, as in Eq. (34), since it propagates down the hierarchy of equations of motion. We report elsewhere the *minimal theory*, where the condition for cancellation is $u_J = -2u_t$, with a relative coefficient 2.

[16] Since finite-T many-body theory formalism is of an isothermal rather than adiabatic character, where quantum numbers are unconstrained and consequently the Fermi surface changes its shape, the conventional usage of the term adiabatic continuity seems misplaced. It might be more appropriately replaced by the term "parametric continuity" or just "continuity."

[17] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).

[18] W. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302 (1970).

[19] G. Baskaran, Z. Zhou, and P. W. Anderson, Solid State Commun. **63**, 973 (1987).

[20] G. Kotliar, Phys. Rev. B **37**, 3664 (1988).