Lecture 8: Strongly correlated electronic systems: Hubbard, periodic Anderson, and Kondo models

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Abstract

The Hubbard, periodic Anderson, and Kondo models are defined. The symmetries of the Hubbard model are derived. The conditions for the ferromagnetic and antiferromagnetic instabilities in the one-band Hubbard model are derived within the random phase approximation.

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I. INTRODUCTION

One of the great mysteries of solid state physics is how does quantum magnetism emerge. If we posit that the theory of everything in solid state physics is the sum of the kinetic energy of electrons and ions together with their mutual Coulomb repulsion, then neither does the kinetic energy favor magnetism and, in particular, ferromagnetism nor does the Coulomb interaction. The very existence of quantum magnetism must however imply that quantum magnetism and, in particular, ferromagnetism can emerge from the competition between the kinetic and the interaction energy.

The Hubbard model was devised by Hubbard as the simplest possible model of itinerant electrons that could display an instability of the Fermi liquid to a ferromagnetic ground state as a result of short-range repulsive interactions, the remnants of the long-range Coulomb interaction. The Hubbard model plays the role in the physics of strong electronic correlations of the Ising model in classical statistical physics. Aside from its pure academic interest, it is believed by some to capture some essential physics responsible for high-temperature superconductivity.

II. A BRIEF REVIEW OF BAND THEORY

Band theory treats all interactions between electrons and all interactions between the electrons and the ions in a solid at the level of an effective periodic one-particle potential $V_{\rm eff}(\mathbf{r})$. Having optimized the choice for $V_{\rm eff}(\mathbf{r})$, a discipline in itself, one is left with the task of solving the eigenvalue problem

$$\begin{bmatrix} -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{eff}}(\mathbf{r}) \end{bmatrix} \phi_{\sigma,n,\mathbf{k}}(\mathbf{r}) = \varepsilon_{n,\mathbf{k}} \phi_{\sigma,n,\mathbf{k}}(\mathbf{r}),$$

$$\int_{L} d^d \mathbf{r} \, \phi^*_{\sigma,n,\mathbf{k}}(\mathbf{r}) \, \phi_{\sigma',n',\mathbf{k}'}(\mathbf{r}) = \delta_{\sigma,\sigma'} \delta_{n,n'} \delta_{\mathbf{k},\mathbf{k}'},$$

$$\sum_{n} \sum_{\mathbf{k}} \phi^*_{\sigma,n,\mathbf{k}}(\mathbf{r}) \, \phi_{\sigma,n,\mathbf{k}}(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}').$$
(2.1)

Here, we are assuming that spin-rotation symmetry (SRS) and time-reversal symmetry (TRS) are present, for simplicity. Thus, the electronic spin quantum number $\sigma = \uparrow, \downarrow$ is a good quantum number. We are also imposing periodic boundary conditions in an hyper-

cubic box of linear size L so that the wave number is quantized

$$\boldsymbol{k} = \frac{2\pi}{L} \boldsymbol{m}, \qquad \boldsymbol{m} \in \mathbb{Z}^d.$$

The range of allowed values \boldsymbol{k} is the number $N_{\rm uc}$ of unit cells in the solid. We restrict all \boldsymbol{k} to the first Brillouin zone (BZ). The quantum number $n \in \mathbb{N}$ then labels the distinct bands. The triplet of quantum number $(\sigma, n, \boldsymbol{k})$ defines a Bloch (single-particle) state. The many-body ground state for $N_{\rm e}$ electrons is the filled Fermi sea (FFS)

$$|\text{FFS}\rangle := \bigwedge_{n} \bigwedge_{\sigma} \bigwedge_{\boldsymbol{k} \in \text{FFS}} |\sigma, n, \boldsymbol{k}\rangle, \qquad \text{FFS} := \bigcup_{n} \left\{ \boldsymbol{k} \in \text{BZ} | \varepsilon_{n, \boldsymbol{k}} \le \varepsilon_{\text{F}} \right\},$$
(2.3)

obtained by filling the $N_{\rm e}$ single-particle Bloch states with the lowest energies up to the Fermi energy $\varepsilon_{\rm F}.$

In band theory, the single-particle density of states (DoS)

$$\nu(\varepsilon) := L^{-d} \sum_{\sigma} \sum_{n} \sum_{k} \delta(\varepsilon - \varepsilon_{n,k})$$
(2.4)

plays a very important role. In the thermodynamic limit, the DoS is generically an analytic function of ε , except for isolated singularities, with a compact support made of a finite union of intervals U_i

$$\operatorname{supp} \nu = \bigcup_{i} U_{i} \tag{2.5}$$

that we assume ordered along the energy axis (see Fig. 1). The energy interval that separates a pair (U_i, U_{i+1}) is called a spectral gap. In simple cases, the index *i* is the same as the band index but this need not always be so as different energy bands can overlap. Each band *n* can accommodate the maximum number of $2N_{\rm uc}$ electrons in the BZ. For nonoverlapping bands, if the number of electrons N_e satisfies the condition that

$$\frac{N_{\rm e}}{2N_{\rm uc}} \in \mathbb{N}$$
(2.6)

is held fixed as the thermodynamic limit $N_{\rm e}, N_{\rm uc} \rightarrow \infty$ is taken, it costs a finite energy to create a particle-hole excitation out of the Fermi sea at zero temperature. This property defines a band insulator. When the largest single-particle energy eigenvalue $\varepsilon_{\rm F}$ is characterized by a nonvanishing DoS $\nu(\varepsilon_{\rm F})$ and when $\varepsilon_{\rm F}$ is inside an energy band, i.e., a finite distance away from the threshold energy to a gap between two bands, it costs an arbitrarily small energy to create a particle-hole excitation out of the Fermi sea at zero temperature. Both



FIG. 1: Generic DoS in band theory

properties define a metal. Many properties of the metallic state are solely controlled by the single-particle states close to the Fermi surface (FS)

$$FS := \bigcup_{\mathbf{r}} \left\{ \boldsymbol{k} \in BZ | \varepsilon_{n, \boldsymbol{k}} = \varepsilon_{F} \right\}.$$
(2.7)

Since we are interested in the effects of the Coulomb repulsion between electrons that cannot be incorporated in the self-consistent single-particle potential $V_{\text{eff}}(\mathbf{r})$, it is indispensable to use the second quantization formulation of quantum mechanics. We assume that we have solved the single-particle eigenvalue problem (2.1). We introduce the Fock space \mathcal{H} as the span of all the states generated from the vacuum $|0\rangle$ by the creation operators $\hat{c}^{\dagger}_{\sigma,n,\mathbf{k}}$ that obey the fermion algebra

$$\{\hat{c}_{\sigma,n,\boldsymbol{k}},\hat{c}_{\sigma',n',\boldsymbol{k}'}^{\dagger}\} = \delta_{\sigma,\sigma'}\delta_{n,n'}\delta_{\boldsymbol{k},\boldsymbol{k}'}, \qquad \{\hat{c}_{\sigma,n,\boldsymbol{k}}^{\dagger},\hat{c}_{\sigma',n',\boldsymbol{k}'}^{\dagger}\} = \{\hat{c}_{\sigma,n,\boldsymbol{k}},\hat{c}_{\sigma',n',\boldsymbol{k}'}^{\dagger}\} = 0.$$
(2.8a)

Define the second-quantized kinetic energy

$$\hat{H}_{\rm kin} := \sum_{\sigma} \sum_{n} \sum_{\boldsymbol{k}} \left(\varepsilon_{n,\boldsymbol{k}} - \mu \right) \hat{c}^{\dagger}_{\sigma,n,\boldsymbol{k}} \hat{c}_{\sigma,n,\boldsymbol{k}} \equiv \sum_{\sigma} \sum_{n} \sum_{\boldsymbol{k}} \xi_{n,\boldsymbol{k}} \hat{c}^{\dagger}_{\sigma,n,\boldsymbol{k}} \hat{c}_{\sigma,n,\boldsymbol{k}}.$$
(2.8b)

The kinetic Hamiltonian (2.8b) can be represented in direct space by

$$\hat{H}_{\rm kin} := \sum_{\sigma} \int_{L^d} d^d \boldsymbol{r} \, \hat{\psi}^{\dagger}_{\sigma}(\boldsymbol{r}) \left(-\frac{\hbar^2}{m^2} \boldsymbol{\partial}^2 - \mu + V_{\rm eff}(\boldsymbol{r}) \right) \hat{\psi}_{\sigma}(\boldsymbol{r}) \tag{2.9a}$$

where we have introduced the creation and annihilation operators

$$\hat{\psi}^{\dagger}_{\sigma}(\boldsymbol{r}) := \sum_{n,\boldsymbol{k}} \phi^{*}_{\sigma,n,\boldsymbol{k}}(\boldsymbol{r}) \, \hat{c}^{\dagger}_{\sigma,n,\boldsymbol{k}} \iff \hat{c}^{\dagger}_{\sigma,n,\boldsymbol{k}} := \int_{L} d^{d}\boldsymbol{r} \, \phi_{\sigma,n,\boldsymbol{k}}(\boldsymbol{r}) \, \hat{\psi}^{\dagger}_{\sigma}(\boldsymbol{r}),
\hat{\psi}_{\sigma}(\boldsymbol{r}) := \sum_{n,\boldsymbol{k}} \phi_{\sigma,n,\boldsymbol{k}}(\boldsymbol{r}) \, \hat{c}_{\sigma,n,\boldsymbol{k}} \iff \hat{c}_{\sigma,n,\boldsymbol{k}} =: \int_{L} d^{d}\boldsymbol{r} \, \phi^{*}_{\sigma,n,\boldsymbol{k}}(\boldsymbol{r}) \, \hat{\psi}_{\sigma}(\boldsymbol{r}),$$

$$(2.9b)$$

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in terms of the single-particle Bloch wave functions. The Bravais lattice is not explicit in this representation. An alternative representation that makes the Bravais lattice $\{R_i\}$ explicit is defined by the Fourier transformation from the Bloch to the Wannier wavefunctions,

$$\phi_{\sigma,n,i}(\boldsymbol{r}) = N_{\mathrm{uc}}^{-1/2} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} \phi_{\sigma,n,\boldsymbol{k}}(\boldsymbol{r}) \Longleftrightarrow \phi_{\sigma,n,\boldsymbol{k}}(\boldsymbol{r}) = N_{\mathrm{uc}}^{-1/2} \sum_i e^{+i\boldsymbol{k}\cdot\boldsymbol{R}_i} \phi_{\sigma,n,i}(\boldsymbol{r}). \quad (2.10)$$

We are thus lead to define the Wannier creation and annihilation operators

$$\hat{c}^{\dagger}_{\sigma,n,i} := \int_{L} d^{d} \boldsymbol{r} \, \phi_{\sigma,n,i}(\boldsymbol{r}) \, \hat{\psi}^{\dagger}_{\sigma}(\boldsymbol{r}) \iff \hat{\psi}^{\dagger}_{\sigma}(\boldsymbol{r}) =: \sum_{n,i} \phi^{*}_{\sigma,n,i}(\boldsymbol{r}) \, \hat{c}^{\dagger}_{\sigma,n,i}, \\
\hat{c}_{\sigma,n,i} := \int_{L} d^{d} \boldsymbol{r} \, \phi^{*}_{\sigma,n,i}(\boldsymbol{r}) \, \hat{\psi}_{\sigma}(\boldsymbol{r}) \iff \hat{\psi}_{\sigma}(\boldsymbol{r}) =: \sum_{n,i} \phi_{\sigma,n,i}(\boldsymbol{r}) \, \hat{c}_{\sigma,n,i}.$$
(2.11)

Wannier creation and annihilation operators are related to Bloch creation and annihilation operators by the Fourier transforms

$$\hat{c}^{\dagger}_{\sigma,n,\boldsymbol{k}} = N_{\mathrm{uc}}^{-1/2} \sum_{i} e^{+i\boldsymbol{k}\cdot\boldsymbol{R}_{i}} \hat{c}^{\dagger}_{\sigma,n,i} \iff \hat{c}^{\dagger}_{\sigma,n,i} = N_{\mathrm{uc}}^{-1/2} \sum_{i} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_{i}} \hat{c}^{\dagger}_{\sigma,n,\boldsymbol{k}},$$

$$\hat{c}_{\sigma,n,\boldsymbol{k}} = N_{\mathrm{uc}}^{-1/2} \sum_{i} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_{i}} \hat{c}_{\sigma,n,i} \iff \hat{c}_{\sigma,n,i} = N_{\mathrm{uc}}^{-1/2} \sum_{i} e^{+i\boldsymbol{k}\cdot\boldsymbol{R}_{i}} \hat{c}_{\sigma,n,\boldsymbol{k}}.$$
(2.12)

They obey the fermion algebra

$$\{\hat{c}_{\sigma,n,i},\hat{c}_{\sigma',n',i'}^{\dagger}\} = \delta_{\sigma,\sigma'}\delta_{n,n'}\delta_{i,i'}, \qquad \{\hat{c}_{\sigma,n,i}^{\dagger},\hat{c}_{\sigma',n',i'}^{\dagger}\} = \{\hat{c}_{\sigma,n,i},\hat{c}_{\sigma',n',i'}\} = 0,$$
(2.13a)

while insertion of Eq. (2.12) into the kinetic Hamiltonian (2.8b) yields

$$\hat{H}_{\rm kin} = -\sum_{\sigma} \sum_{n} \sum_{i,j} \left(t_{n,i,j} + \mu \delta_{ij} \right) \hat{c}^{\dagger}_{\sigma,n,i} \hat{c}_{\sigma,n,j}$$
(2.13b)

where the so-called hopping amplitude between the Bravais sites \mathbf{R}_i and \mathbf{R}_j for band n is given by

$$t_{n,i,j} = -\frac{1}{N_{\rm uc}} \sum_{\boldsymbol{k}} e^{+i\boldsymbol{k}\cdot\left(\boldsymbol{R}_i - \boldsymbol{R}_j\right)} \varepsilon_{n,\boldsymbol{k}} = t^*_{n,j,i}.$$
(2.13c)

The Wannier representation (2.13) of the kinetic energy is a useful starting point when one anticipates or observes that a conducting phase predicted by band theory is destroyed by an effective short-range repulsive two-particle interaction.

III. THE HUBBARD, THE ANDERSON, AND THE KONDO MODELS OF LO-CAL INTERACTIONS

We begin this section by representing the Coulomb interaction

$$\hat{H}_{\rm cb} = \frac{1}{2} \sum_{\sigma,\sigma'} \int_{L^d} d^d \boldsymbol{r} \int_{L^d} d^d \boldsymbol{r'} W_{\rm cb}(\boldsymbol{r} - \boldsymbol{r'}) \, \hat{\psi}^{\dagger}_{\sigma}(\boldsymbol{r}) \hat{\psi}^{\dagger}_{\sigma'}(\boldsymbol{r'}) \hat{\psi}_{\sigma'}(\boldsymbol{r'}) \hat{\psi}_{\sigma}(\boldsymbol{r})$$
(3.1a)

where

$$W_{\rm cb}(\boldsymbol{r} - \boldsymbol{r}') = L^{-d} \sum_{\boldsymbol{q} \neq \boldsymbol{0}} e^{-\mathrm{i}(\boldsymbol{r} - \boldsymbol{r}') \cdot \boldsymbol{q}} \frac{4\pi e^2}{\boldsymbol{q}^2}$$
(3.1b)

in the Wannier basis, namely

$$\hat{H}_{cb} = \frac{1}{2} \sum_{\sigma_1, n_1, i_1} \cdots \sum_{\sigma_4, n_4, i_4} W_{cb\, 1, 2|3, 4} \delta_{\sigma_1, \sigma_3} \delta_{\sigma_2, \sigma_4} \, \hat{c}^{\dagger}_{\sigma_1, n_1, i_1} \hat{c}^{\dagger}_{\sigma_2, n_2, i_2} \hat{c}_{\sigma_4, n_4, i_4} \hat{c}_{\sigma_3, n_3, i_3} \tag{3.2a}$$

where

$$W_{\rm cb\,1,2|3,4} := \int_{L^d} d^d \boldsymbol{r} \int_{L^d} d^d \boldsymbol{r}' \, \phi^*_{\sigma_1,n_1,i_1}(\boldsymbol{r}) \phi_{\sigma_3,n_3,i_3}(\boldsymbol{r}) \, W_{\rm cb}(\boldsymbol{r}-\boldsymbol{r}') \, \phi^*_{\sigma_2,n_2,i_2}(\boldsymbol{r}') \phi_{\sigma_4,n_4,i_4}(\boldsymbol{r}').$$
(3.2b)

We have seen in Lecture 6 that the Coulomb interaction in the jellium model, owing to its long-range nature, causes infrared (IR) singularities when it is treated perturbatively. In the random phase approximation (RPA), these IR singularities could be tamed and it was shown that new collective excitations emerge in the quasidynamic limit (plasmons) while screening is the trademark of the quasistatic limit.

Hubbard defines the (one-band) Hubbard model by truncating the Coulomb interaction in the Wannier basis to a single on-site interaction,

$$\begin{split} \dot{H}_{\text{Hub}} &:= \dot{H}_{\text{kin}} + \dot{H}_{\text{int}}, \\ \dot{H}_{\text{kin}} &:= \sum_{\sigma} \sum_{\boldsymbol{k}} \left(\varepsilon_{\boldsymbol{k}} - \mu \right) \hat{c}^{\dagger}_{\sigma, \boldsymbol{k}} \hat{c}_{\sigma, \boldsymbol{k}} = -\sum_{\sigma} \sum_{\langle i, j \rangle} \left(t \hat{c}^{\dagger}_{\sigma, i} \hat{c}_{\sigma, j} + \text{H.c.} \right) - \mu \sum_{\sigma} \sum_{i} \hat{c}^{\dagger}_{\sigma, i} \hat{c}_{\sigma, i}, \\ \hat{H}_{\text{int}} &:= \frac{U}{N_{\text{uc}}} \sum_{\boldsymbol{q} \neq \boldsymbol{0}} \sum_{\boldsymbol{k}_{1}, \boldsymbol{k}_{2}} c^{\dagger}_{\uparrow, \boldsymbol{k}_{1} + \boldsymbol{q}} c^{\dagger}_{\downarrow, \boldsymbol{k}_{2} - \boldsymbol{q}} c_{\downarrow, \boldsymbol{k}_{2}} c_{\uparrow, \boldsymbol{k}_{1}} = U \left(\sum_{i} \hat{n}_{\uparrow, i} \hat{n}_{\downarrow, i} - \frac{1}{N_{\text{uc}}} \sum_{\boldsymbol{k}_{1}, \boldsymbol{k}_{2}} c^{\dagger}_{\uparrow, \boldsymbol{k}_{1}} c^{\dagger}_{\downarrow, \boldsymbol{k}_{2}} c_{\downarrow, \boldsymbol{k}_{2}} c_{\uparrow, \boldsymbol{k}_{1}} \right), \end{split}$$

$$(3.3a)$$

where $\langle i, j \rangle$ denotes a directed pair of nearest-neighbor sites of the Bravais lattice and

$$\hat{n}_{\sigma,i} := \hat{c}^{\dagger}_{\sigma,i} \hat{c}_{\sigma,i}. \tag{3.3b}$$

The condition of charge neutrality is usually ignored and we will drop the condition $q \neq 0$ in the interaction term from now on unless stated otherwise. The energy scale t > 0 characterizes the strength of the kinetic energy through the band width. The energy scale U > 0 characterizes the repulsive interaction. The foremost justification for this approximation is its simplicity. Second, it is plausible for Wannier single-particle states $\phi_{\sigma,i}(\mathbf{r})$ that decay exponentially fast away from their Bravais lattice \mathbf{R}_i with a small decay (localization) length, an assumption usually made for metals with a small band width of the order of $10^{-2} eV$ such as occurs for the f atomic orbitals in rare earth metals or the d atomic orbitals in transition metals oxide. Third, it is also made plausible by the physics of screening in a good metal if one approaches from the conducting side a putative phase transition driven by the interaction U to a so-called Mott insulating phase. Of course, on the insulating side of a Mott transition, the long-range nature of the Coulomb interaction must be accounted for.

The Hubbard model can be generalized to allow more than one band, longer-range hopping, longer-range interactions, etc. For example, in the field of high-temperature superconductivity, the Bravais lattice is a square or a rectangle and hopping amplitudes up to the third nearest neighbors are accounted for. The periodic Anderson model

$$\hat{H}_{pA} := \sum_{\sigma, \mathbf{k}} \left(\varepsilon_{\mathbf{k}} - \mu \right) \hat{c}^{\dagger}_{\sigma, \mathbf{k}} \hat{c}_{\sigma, \mathbf{k}} + \varepsilon_{f} \sum_{\sigma, \mathbf{k}} \hat{f}^{\dagger}_{\sigma, \mathbf{k}} \hat{f}_{\sigma, \mathbf{k}} + U \sum_{i} \hat{f}^{\dagger}_{\uparrow, i} \hat{f}_{\uparrow, i} \hat{f}^{\dagger}_{\downarrow, i} \hat{f}^{\dagger}_{\downarrow, i} \hat{f}^{\dagger}_{\downarrow, i} \\ - \sum_{\sigma, \mathbf{k}} \left(V_{\mathbf{k}} \hat{c}^{\dagger}_{\sigma, \mathbf{k}} \hat{f}_{\sigma, \mathbf{k}} + \text{H.c.} \right)$$

$$(3.4)$$

describes conduction electrons, denoted by the creation and annihilation operators with the Latin letter c, that interact with localized electrons, denoted by the creation and annihilation operators with the Latin letter f, through the hybridization matrix element V_k . In the limit of very dilute density of f-electrons, the periodic Anderson model is replaced by the Kondo model

$$\hat{H}_{\text{Kondo}} := \sum_{\sigma, \mathbf{k}} \left(\varepsilon_{\mathbf{k}} - \mu \right) \hat{c}^{\dagger}_{\sigma, \mathbf{k}} \hat{c}_{\sigma, \mathbf{k}} + \varepsilon_{\text{f}} \sum_{\sigma} \hat{f}^{\dagger}_{\sigma} \hat{f}_{\sigma} + U \hat{f}^{\dagger}_{\uparrow} \hat{f}_{\uparrow} \hat{f}^{\dagger}_{\downarrow} \hat{f}^{\dagger}_{\downarrow} \\ - N_{\text{uc}}^{-1/2} \sum_{\sigma, \mathbf{k}} \left(V_{\mathbf{k}} \hat{c}^{\dagger}_{\sigma, \mathbf{k}} \hat{f}_{\sigma} + \text{H.c.} \right)$$
(3.5)

in which the conduction electrons interact with a single "impurity".

We shall limit ourselves to the study of the (one-band) Hubbard model (3.3) in this class. The Hubbard model is the simplest model that incorporates the competition between the kinetic energy and a repulsive short-range interaction while accounting for a band structure.

On the one hand, the Pauli principle obeyed by fermions forbids the minimalization of the kinetic energy by the occupation of a single Bloch state by all electrons, i.e., the macroscopic occupation of a single-particle eigenstate as would be the case for bosons. Instead, the wave-like nature of the ground state for the kinetic energy is encoded by the Fermi sea. Moreover, $\hat{H}_{\rm kin}$ quenches the magnetic response. Indeed, the magnetic susceptibility of $\hat{H}_{\rm kin}$ is the product of two terms. There is the factor

$$\chi_{\rm Curie}(T) \propto \frac{\mu_{\rm B}^2}{T} \tag{3.6}$$

that obeys the Curie law for noninteracting spins. There is the factor

$$\frac{T}{\varepsilon_{\rm F}}$$
 (3.7)

that counts the fraction of electron spins available at low temperatures through the Fermi-Dirac distribution. This gives the Pauli susceptibility

$$\chi_{\text{Pauli}}(T) \propto \mu_{\text{B}}^2 \nu(\varepsilon_{\text{F}}) + \mathcal{O}(T/\varepsilon_{\text{F}})$$
 (3.8)

with a weak dependence on temperature at low temperatures.

On the other hand, the Hubbard interaction commutes with the local particle number (3.3b). The ground state of the Hubbard interaction tries to localize a single electron per Bravais lattice site as the local on site energy is

$$U\hat{n}_{\uparrow,i}\hat{n}_{\downarrow,i} = \begin{cases} 0, & \text{if no electron occupies site } i, \\ 0, & \text{if one electron occupies site } i, \\ U, & \text{if two electrons occupies site } i. \end{cases}$$
(3.9)

The intensive magnetic susceptibility of $\hat{H}_{\rm int}$ when $N_{\rm e}/N_{\rm uc} < 2$ thus obeys the Curie law (3.6) with a proportionality constant of order $N_{\rm e}/(2N_{\rm uc})$ if $N_{\rm e}/(2N_{\rm uc}) \ll 1$.

Although neither does the kinetic energy alone nor does the short-range repulsive potential alone favor magnetism, the Pauli principle could lead to ferromagnetism in the following way. When U is large it costs a lot of energy to occupy a site with electrons of opposite spins. By aligning the spin of the electrons double occupancy of sites is avoided and the interaction energy is lowered. Of course this comes at a cost in kinetic energy due to the imbalance in the spin population.



FIG. 2: Parameter space for the fermionic repulsive Hubbard model.

An active research area is to determine the zero-temperature phase diagram of the Hubbard model for a given Bravais lattice when parameter space is labeled by the dimensionless ratio $0 \leq U/t < \infty$ on the horizontal axis and the ratio $0 \leq N_e/(2N_{uc}) \leq 1$ (held fixed in the thermodynamic limit $N_e, N_{uc} \to \infty$) on the vertical axis. The main question that is still evading an answer to this date in dimensions larger than d = 1 is the outcome of this competition between a kinetic energy that favors delocalized electrons with a quenched magnetic response and a correlation energy that favors localized electrons with a magnetic response obeying the Curie law.

IV. SYMMETRIES OF THE HUBBARD MODEL

To review the symmetries of the Hubbard model we use the following definitions. A graph is made of a set of vertices Λ with cardinality $|\Lambda|$ and a set of unordered bonds connecting distinct pairs of these vertices. A graph is more general than a Bravais lattice as it does not require the notion of translation invariance. A Hermitean hopping matrix T with nonvanishing matrix elements t_{ij} whenever $i \in \Lambda$ and $j \in \Lambda$ are connected by a bond is given. By convention $t_{ii} = 0$. The phase of the product of the matrix elements t_{ij} along an oriented closed path of the graph is interpreted as the magnetic flux threading the area enclosed by this path. A real-valued vector U with elements U_i with $i \in \Lambda$ is given. The one-band Hubbard model on the graph with hopping matrix T and real-valued vector U is

the Hermitean Hamiltonian

$$\begin{split} \hat{H}_{T,U} &:= \hat{H}_{\mathrm{kin}} + \hat{H}_{\mathrm{int}}, \\ \hat{H}_{\mathrm{kin}} &:= \sum_{\sigma=\uparrow,\downarrow} \hat{H}_{\mathrm{kin}\,\sigma}, \qquad \hat{H}_{\mathrm{kin}\,\sigma} := -\sum_{i,j\in\Lambda} t_{ij} \, c^{\dagger}_{\sigma,i} c_{\sigma,j}, \\ \hat{H}_{\mathrm{int}} &:= \sum_{i\in\Lambda} U_i \, \left(\hat{n}_{\uparrow,i} - \frac{1}{2} \right) \left(\hat{n}_{\downarrow,i} - \frac{1}{2} \right), \qquad \hat{n}_{\sigma,i} := \hat{c}^{\dagger}_{\sigma,i} \hat{c}_{\sigma,i} \end{split}$$
(4.1a)

acting on the Hilbert space

$$\mathcal{H} = \operatorname{span} \left\{ \prod_{\sigma=\uparrow, \downarrow} \prod_{i \in \Lambda} \left(c_{\sigma,i}^{\dagger} \right)^{m_{\sigma,i}} |0\rangle \middle| c_{\sigma,i} |0\rangle = 0, \qquad m_{\sigma,i} = 0, 1 \right\}.$$
(4.1b)

Comments: The rational for the redefinition of the interaction is that it is left invariant under the transformation

$$\hat{c}^{\dagger}_{\uparrow,i} \rightarrow \hat{c}^{\dagger}_{\uparrow,i}, \qquad \hat{c}_{\uparrow,i} \rightarrow \hat{c}_{\uparrow,i}, \qquad \hat{c}^{\dagger}_{\downarrow,i} \rightarrow \hat{c}_{\downarrow,i}, \qquad \hat{c}_{\downarrow,i} \rightarrow \hat{c}^{\dagger}_{\downarrow,i}, \qquad U_i \rightarrow -U_i \,. \tag{4.2}$$

A graph is bipartite if $\Lambda = A \cup B$ with A and B disjoint and if there are no bonds between i and j whenever i and j both belong to A or B. A square lattice is bipartite. A triangular lattice is not bipartite. The band is half-filled when $N_{\rm e} = |\Lambda|$.

Hamiltonian (4.1a) is left invariant by the global U(1) gauge transformation

$$\hat{c}^{\dagger}_{\sigma,i} \to \hat{c}^{\dagger}_{\sigma,i} e^{-i\chi}, \qquad \hat{c}_{\sigma,i} \to \hat{c}_{\sigma,i} e^{+i\chi}, \qquad \chi \in \mathbb{R}.$$

$$(4.3)$$

Consequently, the total number operator

$$\hat{N}_{\rm e} := \sum_{\sigma} \sum_{i} \hat{n}_{\sigma,i} \tag{4.4}$$

commutes with \hat{H} and its eigenvalue $N_{\rm e}$ is bounded from above by $2|\Lambda|$,

$$0 \le N_e \le 2|\Lambda| \tag{4.5}$$

as each site cannot be occupied by more than two electrons.

Hamiltonian (4.1a) commutes with the global generators

$$\hat{\boldsymbol{S}} \equiv \sum_{i} \hat{\boldsymbol{S}}_{i} := \sum_{i} \sum_{\alpha,\beta} \hat{c}_{\alpha,i}^{\dagger} \frac{\hbar \boldsymbol{\sigma}_{\alpha\beta}}{2} \hat{c}_{\beta,i} = \frac{\hbar}{2} \sum_{i} \begin{pmatrix} c_{\uparrow,i}^{\dagger} c_{\downarrow,i} + c_{\downarrow,i}^{\dagger} c_{\uparrow,i} \\ -i \left(c_{\uparrow,i}^{\dagger} c_{\downarrow,i} - c_{\downarrow,i}^{\dagger} c_{\uparrow,i} \right) \\ c_{\uparrow,i}^{\dagger} c_{\uparrow,i} - c_{\downarrow,i}^{\dagger} c_{\downarrow,i} \end{pmatrix}$$
(4.6)

of the SU(2) spin rotations.

Proof. Let

$$\hat{\boldsymbol{S}}_{i} := \frac{\hbar}{2} \hat{c}_{\alpha,i}^{\dagger} \,\boldsymbol{\sigma}_{\alpha\beta} \,\hat{c}_{\beta,i}, \qquad \hat{n}_{i} := \hat{c}_{\alpha,i}^{\dagger} \,\delta_{\alpha,\beta} \,\hat{c}_{\beta,i}, \tag{4.7}$$

where the summation convention on repeated Greek indices is used. Both \hat{n}_i and the kinetic energy $\hat{H}_{\rm kin}$ in Eq. (4.1a) are SU(2) singlets as they are fermion bilinears built out of $\delta_{\alpha,\beta}$, i.e., they are invariant under the global SU(2) transformation

$$\hat{c}^{\dagger}_{\alpha,i} \to \hat{c}^{\dagger}_{\beta',i} U^*_{\alpha\beta'} \qquad \hat{c}_{\alpha,i} \to U_{\alpha\beta} \hat{c}_{\beta,i}, \qquad U^*_{\alpha\beta'} U_{\alpha\beta} = \delta_{\beta',\beta}.$$
(4.8)

Use the identity

$$\boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{\sigma}_{\alpha'\beta'} = 2\delta_{\alpha,\beta'}\delta_{\beta,\alpha'} - \delta_{\alpha,\beta}\delta_{\alpha',\beta'} \tag{4.9}$$

to prove

$$\begin{split} \hat{\boldsymbol{S}}_{i}^{2} &= \frac{\hbar^{2}}{4} \left(2 \hat{c}_{\alpha,i}^{\dagger} \, \hat{c}_{\beta,i} \, \hat{c}_{\beta,i}^{\dagger} \, \hat{c}_{\alpha,i} - \hat{c}_{\alpha,i}^{\dagger} \, \hat{c}_{\alpha,i} \, \hat{c}_{\alpha',i}^{\dagger} \, \hat{c}_{\alpha',i} \right) \\ &= \frac{\hbar^{2}}{4} \left(4 \hat{n}_{i} \, -3 \hat{n}_{i}^{2} \right) \\ &= \hbar^{2} \left(\frac{1}{4} \hat{n}_{i} \, -\frac{3}{2} \hat{n}_{\uparrow,i} \hat{n}_{\downarrow,i} \right). \end{split}$$
(4.10)

Thus,

$$\begin{split} \hat{H}_{\text{int}} &= \sum_{i \in \Lambda} U_i \, \left(\hat{n}_{\uparrow,i} - \frac{1}{2} \right) \left(\hat{n}_{\downarrow,i} - \frac{1}{2} \right) \\ &= \sum_{i \in \Lambda} U_i \, \left(\hat{n}_{\uparrow,i} \hat{n}_{\downarrow,i} - \frac{1}{2} \hat{n}_i + \frac{1}{4} \right) \\ &= \sum_{i \in \Lambda} U_i \, \left[-\frac{2}{3} \frac{\hat{S}_i^2}{\hbar^2} + \left(\frac{1}{6} - \frac{1}{2} \right) \hat{n}_i + \frac{1}{4} \right] \\ &= \sum_{i \in \Lambda} U_i \, \left(-\frac{2}{3} \frac{\hat{S}_i^2}{\hbar^2} - \frac{1}{3} \hat{n}_i + \frac{1}{4} \right) \end{split}$$
(4.11)

is explicitly an SU(2) singlet as \hat{S}_i^2 represents the Casimir invariant of SU(2).

For a bipartite graph and for a real-valued hopping matrix Hamiltonian (4.1a) is left invariant by the particle-hole transformation

$$\hat{c}^{\dagger}_{\uparrow,i} \to \hat{c}^{\dagger}_{\uparrow,i}, \qquad \hat{c}_{\uparrow,i} \to \hat{c}_{\uparrow,i}, \qquad \hat{c}^{\dagger}_{\downarrow,i} \to \operatorname{sgn}(i) \, \hat{c}_{\downarrow,i}, \qquad \hat{c}_{\downarrow,i} \to \operatorname{sgn}(i) \, \hat{c}^{\dagger}_{\downarrow,i}, \qquad U_i \to -U_i \,,$$

$$(4.12)$$

where $\operatorname{sgn}(i) = +\operatorname{if} i \in A$ and $\operatorname{sgn}(i) = -\operatorname{if} i \in B$.

Proof. Equation (4.2) is still valid under the sign change on sublattice B. The sign change of the kinetic energy for the hopping of the down spin induced by Eq. (4.2) is canceled by the sign change on sublattice B.

Comments: Observe that

$$\hat{N}_{\rm e} \rightarrow \frac{2}{\hbar} \hat{S}_z + |\Lambda|, \qquad \frac{2}{\hbar} \hat{S}_z \rightarrow \hat{N}_{\rm e} - |\Lambda|$$

$$(4.13)$$

under Eq. (4.12). As a corollary to Eq. (4.13) the Hubbard model on a bipartite graph with a real-valued hopping matrix has, in addition to the global SU(2) symmetry (4.6), the global SU(2) pseudospin symmetry generated by

$$\widetilde{\boldsymbol{S}} := \frac{\hbar}{2} \sum_{i} \sum_{\alpha,\beta} \hat{c}^{\dagger}_{\alpha,i} \, \widetilde{\boldsymbol{\sigma}}_{\alpha\beta} \, \hat{c}_{\beta,i} = \frac{\hbar}{2} \sum_{i} \begin{pmatrix} +\operatorname{sgn}(i) \, \left(c^{\dagger}_{\uparrow,i} c^{\dagger}_{\downarrow,i} + c_{\downarrow,i} c_{\uparrow,i} \right) \\ -\operatorname{sgn}(i) i \left(c^{\dagger}_{\uparrow,i} c^{\dagger}_{\downarrow,i} - c_{\downarrow,i} c_{\uparrow,i} \right) \\ c^{\dagger}_{\uparrow,i} c_{\uparrow,i} + c^{\dagger}_{\downarrow,i} c_{\downarrow,i} - 1 \end{pmatrix}.$$
(4.14)

V. RPA ON THE HUBBARD MODEL

To investigate the possible instabilities of the Fermi sea in the Hubbard model to a magnetic ground state, we are going to study the linear response to an external magnetic field. The diagnostic for a magnetic ground state replacing the Fermi sea as the true ground state is that this response becomes infinitely large as one moves across a line in the phase diagram of Fig. 2. We thus need the Kubo formula for the magnetic susceptibility. We will then estimate the magnetic susceptibility within the random phase approximation (RPA).

A. Kubo formula for the magnetic susceptibility

Define the time-dependent Hamiltonian

$$\begin{split} \hat{H}(t) &:= \hat{H}_0 + \Theta(t) \hat{H}'(t), \\ \hat{H}_0 &:= \hat{H}_{T,U}, \\ \hat{H}'(t) &:= -\sum_{i \in \Lambda} \boldsymbol{B}_i(t) \cdot \hat{\boldsymbol{S}}_i. \end{split}$$
(5.1)

We are again using the summation convention for the Greek indices representing the spin-1/2 degree of freedom. The Hubbard Hamiltonian $\hat{H}_{T,U}$ is defined in Eq. (4.1a) with $U_i = U$

and the inclusion of a chemical potential in the kinetic energy so that the dispersion is $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$. The electronic spin operator

$$\hat{\boldsymbol{S}}_{i} = \frac{\hbar}{2} \hat{c}^{\dagger}_{\alpha,i} \,\boldsymbol{\sigma}_{\alpha\beta} \,\hat{c}_{\beta,i} \tag{5.2}$$

was already introduced in Eq. (4.6). According to Lecture 7,

$$\left\langle \hat{S}_{i}^{a}(t) \right\rangle_{0\,\beta,\mu} = \left\langle \hat{S}_{i}^{a} \right\rangle_{0\,\beta,\mu} - \sum_{i'\in\Lambda} \sum_{b=1}^{3} \int_{\mathbb{R}} dt' \,\chi^{a,b}_{\beta,\mu\,ii'}(t-t') B^{b}_{i'}(t'), \tag{5.3a}$$

where

$$\chi^{a,b}_{\beta,\mu\,ii'}(t-t') := -\frac{\mathrm{i}}{\hbar}\Theta(t-t') \left\langle \left[\hat{S}^{a}_{1\,i}(t), \hat{S}^{b}_{1\,i'}(t') \right] \right\rangle_{0\,\beta,\mu}, \qquad a,b = 1, 2, 3.$$
(5.3b)

The Kubo formula in the time and Bravais lattice domains takes the form

$$\left\langle \hat{S}^{a}_{\boldsymbol{q}}(\omega) \right\rangle_{0\,\beta,\mu} = 2\pi \left\langle \hat{S}^{a}_{\boldsymbol{q}} \right\rangle_{0\,\beta,\mu} \delta(\omega) - \sum_{b=1}^{3} \chi^{a,b}_{\beta,\mu\,\boldsymbol{q}}(\omega) B^{b}_{\boldsymbol{q}}(\omega), \tag{5.4a}$$

where

$$\chi^{a,b}_{\beta,\mu\,\boldsymbol{q}}(\omega) = \lim_{\eta\downarrow 0} \int_{\mathbb{D}} dt \, e^{\mathrm{i}(\omega+\mathrm{i}\eta)t} \, \chi^{a,b}_{\beta,\mu\,\boldsymbol{q}}(t) \tag{5.4b}$$

with

$$\chi^{a,b}_{\beta,\mu\,\boldsymbol{q}}(t) = -\frac{\mathrm{i}}{\hbar}\Theta(t)\frac{1}{|\Lambda|}\sum_{\boldsymbol{q}'} \left\langle \left[\hat{S}^{a}_{1\,\boldsymbol{q}}(t),\hat{S}^{b}_{\boldsymbol{q}'}(0)\right]\right\rangle_{0\,\beta,\mu}$$
(5.4c)

and

$$\hat{S}_{q} = \frac{\hbar}{2} \sum_{k \in RZ} \hat{c}^{\dagger}_{\alpha,k+q} \sigma_{\alpha\beta} \hat{c}_{\beta,k} \qquad (5.4d)$$

in the frequency and reciprocal space domains assuming that we have imposed periodic boundary conditions on the Bravais lattice Λ for a translation invariant $\hat{H}_{T,U}$. Here, we are using the Fourier conventions

$$g_{i}(t) = \frac{1}{|\Lambda|} \int_{\mathbb{R}} \frac{d\omega}{2\pi} \sum_{\boldsymbol{k} \in \mathrm{BZ}} e^{+\mathrm{i}\left(\boldsymbol{k} \cdot \boldsymbol{R}_{i} - \omega t\right)} g_{\boldsymbol{k}}(\omega) \Longleftrightarrow g_{\boldsymbol{k}}(\omega) = \int_{\mathbb{R}} dt \sum_{i \in \Lambda} e^{-\mathrm{i}\left(\boldsymbol{k} \cdot \boldsymbol{R}_{i} - \omega t\right)} g_{i}(t) \quad (5.5)$$

for all functions (fermionic creation operators) appearing in the Kubo formula. If SU(2) spin-rotation symmetry is not broken, then

$$\chi^{a,b}_{\beta,\mu\,\boldsymbol{q}}(\omega) = \delta^{a,b}\,\chi_{\beta,\mu\,\boldsymbol{q}}(\omega). \tag{5.6}$$

If SU(2) spin-rotation symmetry is broken, then the magnetic susceptibility is anisotropic with respect to the indices a, b = 1, 2, 3. For the case when the SU(2) spin-rotation symmetry is broken up to rotations generated by \hat{S}^3 , then

$$\chi_{\beta,\mu\,\boldsymbol{q}}^{a,b}(\omega) = \begin{pmatrix} \frac{1}{2}\chi_{\beta,\mu\,\boldsymbol{q}}^{-,+}(\omega) & 0 & 0\\ 0 & \frac{1}{2}\chi_{\beta,\mu\,\boldsymbol{q}}^{-,+}(\omega) & 0\\ 0 & 0 & \chi_{\beta,\mu\,\boldsymbol{q}}^{33}(\omega) \end{pmatrix}$$
(5.7a)

where

$$\chi_{\beta,\mu\boldsymbol{q}}^{-,+}(\omega) := -\frac{\mathrm{i}}{\hbar} \lim_{\eta \downarrow 0} \int_{0}^{\infty} dt \, e^{\mathrm{i}(\omega + \mathrm{i}\eta)t} \, \frac{1}{|\Lambda|} \sum_{\boldsymbol{q}'} \left\langle \left[\hat{S}_{\boldsymbol{\Gamma}\boldsymbol{q}}^{-}(t), \hat{S}_{\boldsymbol{q}'}^{+}(0) \right] \right\rangle_{0\,\beta,\mu} \tag{5.7b}$$

and

$$\hat{S}_{i}^{+} := \hat{S}_{i}^{1} + i\hat{S}_{i}^{2} = \left(\hat{S}_{i}^{-}\right)^{\dagger} = \hbar \, \hat{c}_{\uparrow,i}^{\dagger} \hat{c}_{\downarrow,i}.$$
(5.8)

B. RPA for the magnetic susceptibility

The interaction in the Hubbard model (4.1a) is a two-particle interaction. It can be treated perturbatively as we did with the Coulomb interaction in Lectures 4, 5, and 6 with the simplification that no IR divergences occur order by order in perturbation theory. This is not to say that the Fermi sea is stable as we shall illustrate within the RPA.

As we have seen in Homework 6, the RPA amounts to a particular decoupling of the interaction into an effective one-particle potential. This decoupling is not unique as is suggested by rewriting the Hubbard interaction (4.11) as

$$\hat{H}_{\text{int}} = \sum_{i \in \Lambda} U_i \left(\hat{n}_{\uparrow,i} - \frac{1}{2} \right) \left(\hat{n}_{\downarrow,i} - \frac{1}{2} \right)$$

$$= \sum_{i \in \Lambda} U_i \left[\frac{1}{2} \left(\hat{n}_{\uparrow,i} + \hat{n}_{\downarrow,i} \right)^2 - \left(\hat{n}_{\uparrow,i} + \hat{n}_{\downarrow,i} \right) + \frac{1}{4} \right]$$
(5.9a)

if one wants to emphasize an instability triggered by a charge density wave with the order parameter

$$\left\langle \left(\hat{n}_{\uparrow,i} + \hat{n}_{\downarrow,i} \right) \right\rangle_{0\,\beta,\mu} \tag{5.9b}$$

or

$$\hat{H}_{int} = \sum_{i \in \Lambda} U_i \left(\hat{n}_{\uparrow,i} - \frac{1}{2} \right) \left(\hat{n}_{\downarrow,i} - \frac{1}{2} \right)$$
$$= \sum_{i \in \Lambda} U_i \left[\frac{1}{4} - \frac{1}{2} \left(\hat{n}_{\uparrow,i} - \hat{n}_{\downarrow,i} \right)^2 \right]$$
(5.10a)

if one wants to emphasize an instability triggered by a spin-density wave with the order parameter

$$\left\langle \left(\hat{n}_{\uparrow,i} - \hat{n}_{\downarrow,i}\right) \right\rangle_{0\,\beta,\mu}$$
 (5.10b)

 or

$$\hat{H}_{\text{int}} = \sum_{i \in \Lambda} U_i \left(\hat{n}_{\uparrow,i} - \frac{1}{2} \right) \left(\hat{n}_{\downarrow,i} - \frac{1}{2} \right)
= \sum_{i \in \Lambda} U_i \left[\frac{1}{4} \left(\hat{n}_{\uparrow,i} + \hat{n}_{\downarrow,i} \right)^2 - \frac{1}{4} \left(\hat{n}_{\uparrow,i} - \hat{n}_{\downarrow,i} \right)^2 - \frac{1}{2} \left(\hat{n}_{\uparrow,i} + \hat{n}_{\downarrow,i} \right) + \frac{1}{4} \right]$$
(5.11)

if one wants to treat the charge-density channel on equal footing with the spin-density channel.

Interested as we are by the potential instability of the Fermi sea to a magnetically ordered phase, we decouple the quartic interaction with the spin-density wave order parameter (5.10). Correspondingly, we perform the RPA on the susceptibility (5.7b). If we ignore the spin labels, this is the same susceptibility as the one entering the density-density correlation functions. On this basis, one can make the educated guess that $(\hbar = 1)$

$$\chi_{\beta,\mu\,\boldsymbol{q}}^{-,+\operatorname{rpa}}(\omega) = -\frac{\Gamma_{0\beta,\mu\,\boldsymbol{q}}^{-,+}(\omega)}{1 - U\,\Gamma_{0\beta,\mu\,\boldsymbol{q}}^{-,+}(\omega)},$$

$$\Gamma_{0\beta,\mu\,\boldsymbol{q}}^{-,+}(\omega) := -\frac{1}{|\Lambda|} \sum_{\boldsymbol{k}\in\mathrm{BZ}} \frac{f_{\mathrm{FD}}(\xi_{\uparrow,\boldsymbol{k}}) - f_{\mathrm{FD}}(\xi_{\downarrow,\boldsymbol{k}+\boldsymbol{q}})}{\omega + \xi_{\downarrow,\boldsymbol{k}} - \xi_{\uparrow,\boldsymbol{k}+\boldsymbol{q}} + \mathrm{i}\eta}$$
(5.12a)

where

$$\xi_{\sigma,\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}} - \mu + \frac{U}{|\Lambda|} \sum_{\boldsymbol{k}' \in \mathrm{BZ}} f_{\mathrm{FD}}(\xi_{\sigma,\boldsymbol{k}'}), \qquad \sigma = \uparrow, \downarrow.$$
(5.12b)

We shall derive this result using the method of the equations of motion in appendix A.

C. The instability criterion

We work at sufficiently high temperatures for there not to be a magnetic instability, i.e.,

$$f_{\rm FD}(\xi_{\sigma,\boldsymbol{k}}) = f_{\rm FD}(\xi_{\boldsymbol{k}}), \qquad \Gamma_{0\beta,\mu\,\boldsymbol{q}}^{-,+}(\omega) = \Gamma_{0\beta,\mu\,\boldsymbol{q}}(\omega). \tag{5.13}$$

Magnetic instabilities are singularities of the (RPA) magnetic susceptibilities. They can occur as poles or branch cuts. Branch cuts signal a continuum of excitations. Poles signal a dispersing collective excitation. In the paramagnetic phase, magnetic excitations are heavily damped, i.e., the magnetic susceptibility is a regular function of momentum and frequency. An instability of the paramagnetic phase takes place when the magnetic susceptibility displays a pole at zero frequency, i.e., in the static limit. The wave vector at which the pole occurs defines the magnetic ordering. The instability criterion is thus

$$1 = U \Gamma_{0\beta,\mu q}(\omega = 0). \tag{5.14}$$

in the RPA approximation (5.12).

The so-called Stoner criterion is the special case when the criterion (5.14) is satisfied at the ferromagnetic wave vector q = 0. If we expand the numerator and the denominator of

$$\Gamma_{0\beta,\mu\,\boldsymbol{q}}(\omega=0) = -\frac{1}{|\Lambda|} \sum_{\boldsymbol{k}\in\mathrm{BZ}} \frac{f_{\mathrm{FD}}(\boldsymbol{\xi}_{\boldsymbol{k}}) - f_{\mathrm{FD}}(\boldsymbol{\xi}_{\boldsymbol{k}+\boldsymbol{q}})}{\boldsymbol{\xi}_{\boldsymbol{k}} - \boldsymbol{\xi}_{\boldsymbol{k}+\boldsymbol{q}}}$$
(5.15)

in powers of q and approximate the derivative of the Fermi-Dirac distribution by the delta function, an approximation good when the temperature is much smaller than the Fermi energy, we get the Stoner criterion

$$1 = U \nu(\varepsilon_{\rm F}) \tag{5.16}$$

for the onset of ferromagnetism in the phase diagram of Fig. 2.

Whereas a critical strength of U is needed at a fixed Fermi energy (electron density) for ferromagnetism to be favored, the band structure can favor instabilities at nonvanishing wave vectors \boldsymbol{q} . For example, assume that there exists a special value of \boldsymbol{Q} such that the so-called nesting condition

$$\xi_k = -\xi_{k+Q} \tag{5.17}$$

holds for all \boldsymbol{k} in the BZ. An example is shown in Fig. 3 for the band

$$\varepsilon_{\boldsymbol{k}} = -2t \left(\cos k_x + \cos k_y \right) \tag{5.18}$$

at half-filling when $\boldsymbol{Q} = (\pi, \pi)$. If so

$$\Gamma_{0\,\beta,\mu\,\boldsymbol{Q}}(\omega=0) = -\frac{1}{|\Lambda|} \sum_{\boldsymbol{k}\in\mathrm{BZ}} \frac{f_{\mathrm{FD}}(+\xi_{\boldsymbol{k}}) - f_{\mathrm{FD}}(-\xi_{\boldsymbol{k}})}{2\xi_{\boldsymbol{k}}}$$
$$= \frac{1}{|\Lambda|} \sum_{\boldsymbol{k}\in\mathrm{BZ}} \frac{\tanh\left(\beta\xi_{\boldsymbol{k}}/2\right)}{2\xi_{\boldsymbol{k}}}$$
$$= \int_{\mathbb{R}} d\xi\,\nu(\xi)\,\frac{\tanh\left(\beta\xi/2\right)}{2\xi}.$$

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In the limit of large temperatures

$$\Gamma_{0\beta,\mu}\boldsymbol{\varrho}(\omega=0) \approx \frac{\beta}{4} \int_{\mathbb{R}} d\xi \,\nu(\xi)$$
(5.20)

is finite. In the limit of zero temperature,

$$\Gamma_{0\beta,\mu}\boldsymbol{\varrho}(\omega=0) = \int\limits_{\mathbb{R}} d\xi \frac{\nu(\xi)}{2|\xi|}$$
(5.21)

diverges logarithmically provided the DoS at the Fermi level $\nu_{\rm F}$ is finite. This divergences guarantees that the instability criterion (5.14) is reached for any value of U at the wave vector Q as the temperature is lowered, in contrast to the Stoner criterion for ferromagnetism (5.16) that requires a finite U. For the band (5.18) with the two-dimensional antiferomagnetic ordering wave vector

$$\boldsymbol{Q} = (\pi, \pi) \tag{5.22}$$

the logarithmic divergence (5.21) for a finite DoS at the Fermi energy is enhanced by the fact that the DoS itself diverges logarithmically as

$$\nu(\xi) \sim \ln(t/|\xi|) \tag{5.23}$$

close to the Fermi energy $\xi=0$ at half-filling. This gives the estimate

$$\Gamma_{0\,\beta,\mu\,\boldsymbol{Q}}(\omega=0) \sim \left[\ln(\beta t)\right]^2 \tag{5.24}$$

in the limit of zero temperature [use the integral $\int dx x^{-1} (\ln x)^2 = (1/2) (\ln x)^2$].

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FIG. 3: First Brillouin zone (BZ) of the square lattice is colored in cyan. The Fermi sea at halffilling (one electron per unit cell) is colored in pink. The Fermi surface is a diamond that satisfies the condition of nesting.

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APPENDIX A: PROOF OF EQ. (5.12)

Given the definition

$$\chi_{\beta,\mu}^{-,+}(t) = -\frac{\mathrm{i}}{\hbar}\Theta(t)\left\langle \left[\hat{S}_{1q}^{-}(t), \hat{S}_{1}^{+}(\boldsymbol{x}'=\boldsymbol{0}, t'=0)\right]\right\rangle_{0\,\beta,\mu}$$
(A1a)

where

$$\hat{S}_{1\boldsymbol{q}}^{-}(t) = e^{+\mathrm{i}\hat{H}_{T,U}t/\hbar} \left(\hbar \sum_{\boldsymbol{p}} \hat{c}_{\perp,\boldsymbol{p}+\boldsymbol{q}}^{\dagger} \hat{c}_{\uparrow,\boldsymbol{p}}\right) e^{-\mathrm{i}\hat{H}_{T,U}t/\hbar}$$
(A1b)

and

$$\begin{split} \hat{H}_{T,U} &= \hat{H}_T + \hat{H}_U, \\ \hat{H}_T &= \sum_{\sigma = \uparrow,\downarrow} \sum_{\mathbf{k} \in \mathrm{BZ}} \xi_{\mathbf{k}} \hat{c}^{\dagger}_{\sigma,\mathbf{k}} \hat{c}_{\sigma,\mathbf{k}}, \\ \hat{H}_U &= \frac{U}{|\Lambda|} \sum_{\mathbf{l},\mathbf{k}_1,\mathbf{k}_2 \in \mathrm{BZ}} \hat{c}^{\dagger}_{\uparrow,\mathbf{k}_1+\mathbf{l}} \hat{c}^{\dagger}_{\downarrow,\mathbf{k}_2-\mathbf{l}} \hat{c}_{\downarrow,\mathbf{k}_2} \hat{c}_{\uparrow,\mathbf{k}_1}, \end{split}$$
(A1c)

we have the time derivative

$$\begin{split} \mathrm{i}\hbar\partial_t \chi^{-,+}_{\beta,\mu\,\boldsymbol{q}}(t) &= \delta(t) \left\langle \left[\hat{S}^-_{\boldsymbol{q}}, \hat{S}^+(\boldsymbol{x}'=\boldsymbol{0}) \right] \right\rangle_{0\,\beta,\mu} \\ &- \frac{\mathrm{i}}{\hbar} \Theta(t) \left\langle \left[\left[\hat{S}^-_{1\boldsymbol{q}}(t), \hat{H}_{T,U} \right], \hat{S}^+(\boldsymbol{x}'=\boldsymbol{0}) \right] \right\rangle_{0\,\beta,\mu} \end{split}$$
(A1d)

Comment: We are dropping from the Hubbard interaction (4.1a) with $U_i = U$ the term proportional to the total fermion number and the overall constant without loss of generality. The former contribution amounts to a redefinition of the chemical potential. The latter contribution is an overall constant shift of the energy spectrum that does not affect the linear response. From now on, summations in the BZ are implicit. We shall make the RPA Ansatz for the ground state, namely that

$$\left\langle \hat{c}^{\dagger}_{\sigma,\boldsymbol{k}}\hat{c}_{\sigma',\boldsymbol{k}'}\right\rangle_{0\,\beta,\mu} = \delta_{\sigma,\sigma'}\delta_{\boldsymbol{k},\boldsymbol{k}'}\,f_{\rm FD}(\xi_{\sigma,\boldsymbol{k}}). \tag{A2}$$

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Define

$$\begin{split} \chi_{\beta,\mu\boldsymbol{p},\boldsymbol{q}}^{-,+}(t) &=: \sum_{\boldsymbol{p}} \chi_{\beta,\mu\boldsymbol{p},\boldsymbol{q}}^{-,+}(t), \\ \chi_{\beta,\mu\boldsymbol{p},\boldsymbol{q}}^{-,+}(t) &= -\mathrm{i}\Theta(t) \left\langle \left[\hat{c}^{\dagger}_{\mathbf{l}\downarrow,\boldsymbol{p}+\boldsymbol{q}}(t) \hat{c}_{\mathbf{l}\uparrow,\boldsymbol{p}}(t), \hat{S}^{+}(\boldsymbol{x}'=\boldsymbol{0}) \right] \right\rangle_{0\,\beta,\mu}. \end{split}$$
(A3a)

We have the time derivative

$$\begin{split} \mathrm{i}\hbar\partial_t \chi^{-,+}_{\beta,\mu\,\boldsymbol{p},\boldsymbol{q}}(t) &= \delta(t)\,\hbar\left\langle \left[\hat{c}^{\dagger}_{\downarrow,\boldsymbol{p}+\boldsymbol{q}}\hat{c}_{\uparrow,\boldsymbol{p}},\hat{S}^+(\boldsymbol{x}'=\boldsymbol{0})\right]\right\rangle_{0\,\beta,\mu} \\ &-\mathrm{i}\Theta(t)\left\langle \left[\left[\hat{c}^{\dagger}_{\downarrow,\boldsymbol{p}+\boldsymbol{q}}\hat{c}_{\uparrow,\boldsymbol{p}},\hat{H}_{T,U}\right]_{\mathrm{I}}(t),\hat{S}^+(\boldsymbol{x}'=\boldsymbol{0})\right]\right\rangle_{0\,\beta,\mu}. \end{split}$$
(A3b)

Needed is the coefficient of the delta function in time on the right-hand side of Eq. (A3b)

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$$\begin{split} \left\langle \left[\hat{c}^{\dagger}_{\downarrow,p+q} \hat{c}_{\uparrow,p}, \hat{S}^{+}(\boldsymbol{x}'=\boldsymbol{0}) \right] \right\rangle_{0\,\beta,\mu} &= \frac{\hbar}{|\Lambda|} \left\langle \left[\hat{c}^{\dagger}_{\downarrow,p+q} \hat{c}_{\uparrow,p}, \sum_{\boldsymbol{p}',q'} \hat{c}^{\dagger}_{\uparrow,p'+q'} \hat{c}_{\downarrow,p'} \right] \right\rangle_{0\,\beta,\mu} \\ &= \frac{\hbar}{|\Lambda|} \sum_{\boldsymbol{p}',q'} \left\langle \left(\hat{c}^{\dagger}_{\downarrow,p+q} \hat{c}_{\uparrow,p'} \hat{c}^{\dagger}_{\uparrow,p'+q'} \hat{c}_{\downarrow,p'} - \hat{c}^{\dagger}_{\uparrow,p'+q'} \hat{c}_{\downarrow,p'} \hat{c}^{\dagger}_{\downarrow,p'} \hat{c}_{\uparrow,p} \right) \right\rangle_{0\,\beta,\mu} \\ &= \frac{\hbar}{|\Lambda|} \sum_{\boldsymbol{p}',q'} \left\langle \left(\hat{c}^{\dagger}_{\downarrow,p+q} \hat{c}_{\uparrow,p'+q'} \hat{c}_{\downarrow,p'} \hat{c}^{\dagger}_{\uparrow,p'+q'} \hat{c}_{\downarrow,p'} \hat{c}^{\dagger}_{\uparrow,p'+q'} \hat{c}_{\downarrow,p'} \hat{c}^{\dagger}_{\uparrow,p'+q'} \hat{c}_{\downarrow,p'} \hat{c}^{\dagger}_{\uparrow,p} \right) \right\rangle_{0\,\beta,\mu} \\ &+ \frac{\hbar}{|\Lambda|} \sum_{\boldsymbol{q}'} \left\langle \left(\hat{c}^{\dagger}_{\downarrow,p+q} \hat{c}_{\downarrow,p-q'} - \hat{c}^{\dagger}_{\uparrow,p+q+q'} \hat{c}_{\uparrow,p} \right) \right\rangle_{0\,\beta,\mu} \\ &= \frac{\hbar}{|\Lambda|} \left\langle \left(\hat{c}^{\dagger}_{\downarrow,p+q} \hat{c}_{\downarrow,p+q} - \hat{c}^{\dagger}_{\uparrow,p} \hat{c}_{\uparrow,p} \right) \right\rangle_{0\,\beta,\mu} . \end{split}$$
(A4)

With the help of the RPA Ansatz (A2), we thus find

$$\left\langle \left[\hat{c}^{\dagger}_{\downarrow,\boldsymbol{p}+\boldsymbol{q}} \hat{c}_{\uparrow,\boldsymbol{p}}, \hat{S}^{+}(\boldsymbol{x}'=\boldsymbol{0}) \right] \right\rangle_{0\,\beta,\mu} = \frac{\hbar}{|\Lambda|} \left[f_{\rm FD}(\xi_{\downarrow,\boldsymbol{p}+\boldsymbol{q}}) - f_{\rm FD}(\xi_{\uparrow,\boldsymbol{p}}) \right]. \tag{A5}$$

Needed is the coefficient of the Heaviside function on the right-hand side of Eq. (A3b).

To this end, we need two commutators. First, there is

$$\begin{bmatrix} \hat{c}_{\perp,p+q}^{\dagger}\hat{c}_{\uparrow,p}, \hat{H}_{T} \end{bmatrix} = \sum_{k} \xi_{k} \begin{bmatrix} \hat{c}_{\perp,p+q}^{\dagger}\hat{c}_{\uparrow,p}, \hat{c}_{\sigma,k}^{\dagger}\hat{c}_{\sigma,k}, \end{bmatrix}$$

$$\equiv \sum_{k} \xi_{k} [AB, CD]$$

$$= \sum_{k} \xi_{k} (A [B, CD] + [A, CD] B)$$

$$= \sum_{k} \xi_{k} (A \{B, C\} D - AC \{B, D\} + \{A, C\} DB - C \{A, D\} B)$$

$$= \xi_{p} \hat{c}_{\perp,p+q}^{\dagger}\hat{c}_{\uparrow,p} - \xi_{p+q} \hat{c}_{\uparrow,p+q}^{\dagger}\hat{c}_{\uparrow,p}$$

$$= (\xi_{p} - \xi_{p+q}) \hat{c}_{\perp,p+q}^{\dagger}\hat{c}_{\uparrow,p}.$$

$$(A6)$$

This gives, with the help of Eq. (A3a),

$$-\mathrm{i}\Theta(t)\left\langle \left[\left[\hat{c}_{\downarrow,\boldsymbol{p}+\boldsymbol{q}}^{\dagger}\hat{c}_{\uparrow,\boldsymbol{p}},\hat{H}_{T} \right]_{\mathrm{I}}(t),\hat{S}^{+}(\boldsymbol{x}'=\boldsymbol{0}) \right] \right\rangle_{0\,\beta,\mu}^{\mathrm{RPA}} = \left(\xi_{\boldsymbol{p}} - \xi_{\boldsymbol{p}+\boldsymbol{q}} \right) \chi_{\beta,\mu\,\boldsymbol{p},\boldsymbol{q}}^{-,+\,\mathrm{rpa}}(t). \tag{A7}$$

Second, there is

$$\begin{split} \left[\hat{c}_{\perp,p+q}^{\dagger} \hat{c}_{\uparrow,p}, \hat{H}_{U} \right] &= \frac{U}{|\mathbf{A}|} \sum_{\mathbf{i},\mathbf{k}_{\perp},\mathbf{k}_{\perp}} \left[\hat{c}_{\perp,p+q}^{\dagger} \hat{c}_{\uparrow,p}, \hat{c}_{\uparrow,\mathbf{k}_{\perp}+l}^{\dagger} \hat{c}_{\perp,\mathbf{k}_{2}-l}^{\dagger} \hat{c}_{\perp,\mathbf{k}_{2}} \hat{c}_{\uparrow,\mathbf{k}_{\perp}} \right] \\ &= \frac{U}{|\mathbf{A}|} \sum_{\mathbf{i},\mathbf{k}_{\perp},\mathbf{k}_{\perp}} \left[AB, CDEF \right] \\ &= \frac{U}{|\mathbf{A}|} \sum_{\mathbf{i},\mathbf{k}_{\perp},\mathbf{k}_{\perp}} \left(A \left[B, CDEF \right] + \left[A, CDEF \right] B \right) \right] \\ &= \frac{U}{|\mathbf{A}|} \sum_{\mathbf{i},\mathbf{k}_{\perp},\mathbf{k}_{\perp}} \left(A \left\{ B, CDEF \right\} + \left[A, CDEF \right] B \right) \right] \\ &= \frac{U}{|\mathbf{A}|} \sum_{\mathbf{i},\mathbf{k}_{\perp},\mathbf{k}_{\perp}} \left(A \left\{ B, C \right\} DEF - \underbrace{AC \left\{ B, D \right\} EF}_{=0} + CD \left[A, EF \right] B + \underbrace{[A, CD] EFB}_{=0} \right) \\ &= \frac{U}{|\mathbf{A}|} \sum_{\mathbf{i},\mathbf{k}_{\perp},\mathbf{k}_{\perp}} \left(A \left\{ B, C \right\} DEF - \underbrace{AC \left\{ B, D \right\} EF}_{=0} + CD \left\{ A, E \right\} FB - \underbrace{CDE \left\{ A, F \right\} B}_{=0} \right) \\ &= \frac{U}{|\mathbf{A}|} \sum_{\mathbf{i},\mathbf{k}_{\perp},\mathbf{k}_{\perp}} \left(\delta_{p,\mathbf{k}_{\perp}+l} \hat{c}_{\perp,p+q}^{\dagger} \hat{c}_{\perp,\mathbf{k}_{\perp}-l}^{\dagger} \hat{c}_{\perp,\mathbf{k}_{\perp}} \hat{c}_{\perp,\mathbf{k}_{\perp}-l} \hat{c}_{\perp,\mathbf{k}_{\perp}-l}$$

To close the equation of motion obeyed by $\chi^{-,+}_{\beta,\mu p,q}(t)$ we do the RPA

$$+\hat{c}^{\dagger}_{\downarrow,\boldsymbol{p}+\boldsymbol{q}}\hat{c}_{\uparrow,\boldsymbol{p}-\boldsymbol{l}}\hat{c}^{\dagger}_{\downarrow,\boldsymbol{k}-\boldsymbol{l}}\hat{c}_{\downarrow,\boldsymbol{k}} \rightarrow \left\langle \hat{c}^{\dagger}_{\downarrow,\boldsymbol{p}+\boldsymbol{q}}\hat{c}_{\downarrow,\boldsymbol{k}} \right\rangle_{0\,\beta,\mu}\hat{c}_{\uparrow,\boldsymbol{p}-\boldsymbol{l}}\hat{c}^{\dagger}_{\downarrow,\boldsymbol{k}-\boldsymbol{l}} + \left\langle \hat{c}^{\dagger}_{\downarrow,\boldsymbol{k}-\boldsymbol{l}}\hat{c}_{\downarrow,\boldsymbol{k}} \right\rangle_{0\,\beta,\mu}\hat{c}^{\dagger}_{\downarrow,\boldsymbol{p}+\boldsymbol{q}}\hat{c}_{\uparrow,\boldsymbol{p}-\boldsymbol{l}} \quad (A9)$$

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for the first term on the right-hand side of Eq. (A8) and we do the RPA $\,$

$$-\hat{c}^{\dagger}_{\uparrow,\boldsymbol{k}+\boldsymbol{l}}\hat{c}_{\uparrow,\boldsymbol{k}}\hat{c}^{\dagger}_{\downarrow,\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{l}}\hat{c}_{\uparrow,\boldsymbol{p}} \rightarrow -\left\langle\hat{c}^{\dagger}_{\uparrow,\boldsymbol{k}+\boldsymbol{l}}\hat{c}_{\uparrow,\boldsymbol{k}}\right\rangle_{0\,\beta,\mu}\hat{c}^{\dagger}_{\downarrow,\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{l}}\hat{c}_{\uparrow,\boldsymbol{p}} - \left\langle\hat{c}^{\dagger}_{\uparrow,\boldsymbol{k}+\boldsymbol{l}}\hat{c}_{\uparrow,\boldsymbol{p}}\right\rangle_{0\,\beta,\mu}\hat{c}_{\uparrow,\boldsymbol{k}}\hat{c}^{\dagger}_{\downarrow,\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{l}}$$
(A10)

for the second term on the right-hand side of Eq. (A8). With the help of the RPA Ansatz (A2), we thus find

$$\begin{bmatrix} \hat{c}_{\downarrow,p+q}^{\dagger}\hat{c}_{\uparrow,p}, \hat{H}_{U} \end{bmatrix} = \frac{U}{|\Lambda|} \sum_{l,k} \begin{bmatrix} -\underline{f_{\rm FD}}(\xi_{\downarrow,p+q})\delta_{k,p+q}\hat{c}_{\downarrow,p+q-l}^{\dagger}\hat{c}_{\uparrow,p-l} + \underline{f_{\rm FD}}(\xi_{\downarrow,k})\delta_{l,0}\hat{c}_{\downarrow,p+q}^{\dagger}\hat{c}_{\uparrow,p}}{H} \end{bmatrix}$$

$$+ \frac{U}{|\Lambda|} \sum_{l,k} \begin{bmatrix} -\underline{f_{\rm FD}}(\xi_{\uparrow,k})\delta_{l,0}\hat{c}_{\downarrow,p+q}^{\dagger}\hat{c}_{\uparrow,p}}{H} + \underline{f_{\rm FD}}(\xi_{\uparrow,p})\delta_{k,p-l}\hat{c}_{\downarrow,p+q-l}\hat{c}_{\uparrow,p-l} \end{bmatrix}$$

$$p_{-l \to k'} = \begin{bmatrix} f_{\rm FD}(\xi_{\uparrow,p}) - f_{\rm FD}(\xi_{\downarrow,p+q}) \end{bmatrix} \frac{U}{|\Lambda|} \sum_{k'} \hat{c}_{\downarrow,k'+q}^{\dagger}\hat{c}_{\uparrow,k'}$$

$$+ \begin{cases} \frac{U}{|\Lambda|} \sum_{k} \begin{bmatrix} f_{\rm FD}(\xi_{\downarrow,k}) - f_{\rm FD}(\xi_{\uparrow,k}) \end{bmatrix} \\ \frac{\hat{c}_{\downarrow,p+q}\hat{c}_{\uparrow,p}}{H} \end{bmatrix} \frac{\hat{c}_{\downarrow,p+q}\hat{c}_{\uparrow,p}}{H}$$

$$(A11)$$

The term underlined once does not depend on p since p can be absorbed in a redefinition of the dummy summation index. Hence, with the help of Eq. (A3a),

$$-i\Theta(t)\left\langle \left[\left[\hat{c}_{\downarrow,\boldsymbol{p}+\boldsymbol{q}}^{\dagger}\hat{c}_{\uparrow,\boldsymbol{p}}, \hat{H}_{U} \right]_{I}(t), \hat{S}^{+}(\boldsymbol{x}'=\boldsymbol{0}) \right] \right\rangle_{0,\beta,\mu}^{\text{RPA}} = \left\{ \frac{U}{|\Lambda|} \sum_{\boldsymbol{k}} \left[f_{\text{FD}}(\xi_{\downarrow,\boldsymbol{k}}) - f_{\text{FD}}(\xi_{\uparrow,\boldsymbol{k}}) \right] \right\} \underline{\chi_{\beta,\mu,\boldsymbol{p},\boldsymbol{q}}^{-,+\,\text{rpa}}(t)} + \left[f_{\text{FD}}(\xi_{\uparrow,\boldsymbol{p}}) - f_{\text{FD}}(\xi_{\downarrow,\boldsymbol{p}+\boldsymbol{q}}) \right] \frac{U}{|\Lambda|} \sum_{\boldsymbol{k}} \underline{\chi_{\beta,\mu,\boldsymbol{k},\boldsymbol{q}}^{-,+\,\text{rpa}}(t)}.$$
(A12)

We combine Eqs. (A3b), (A5), (A7), (A12), and (A3a) to obtain the equation of motion in the RPA $\,$

$$\begin{split} \mathrm{i}\hbar\partial_{t}\chi_{\beta,\mu\mathbf{p},\mathbf{q}}^{-,+\mathrm{rpa}}(t) &= \delta(t)\,\hbar\,\frac{\hbar}{|\Lambda|}\left[f_{\mathrm{FD}}(\xi_{\downarrow,\mathbf{p}+\mathbf{q}}) - f_{\mathrm{FD}}(\xi_{\uparrow,\mathbf{p}})\right] \\ &+ \left(\xi_{\mathbf{p}} - \xi_{\mathbf{p}+\mathbf{q}} + \frac{U}{|\Lambda|}\sum_{\mathbf{k}}\left[f_{\mathrm{FD}}(\xi_{\downarrow,\mathbf{k}}) - f_{\mathrm{FD}}(\xi_{\uparrow,\mathbf{k}})\right]\right)\underline{\chi_{\beta,\mu\mathbf{p},\mathbf{q}}^{-,+\mathrm{rpa}}(t)} \\ &+ \left[f_{\mathrm{FD}}(\xi_{\uparrow,\mathbf{p}}) - f_{\mathrm{FD}}(\xi_{\downarrow,\mathbf{p}+\mathbf{q}})\right]\frac{U}{|\Lambda|}\underline{\chi_{\beta,\mu\mathbf{q}}^{-,+\mathrm{rpa}}(t)}. \end{split}$$
(A13)

Define the single-particle Hartree-Fock energy

$$\xi_{\sigma,\boldsymbol{p}} := \xi_{\boldsymbol{p}} + \frac{U}{|\Lambda|} \sum_{\boldsymbol{k}} f_{\rm FD}(\xi_{\sigma,\boldsymbol{k}}), \qquad \sigma = \uparrow, \downarrow.$$
(A14)

With the Fourier convention (5.4b) and with Eq. (A14), Eq. (A13) becomes

$$\left[\hbar\left(\omega+\mathrm{i}\eta\right)+\xi_{\uparrow,\boldsymbol{p}+\boldsymbol{q}}-\xi_{\downarrow,\boldsymbol{p}}\right]\chi_{\beta,\mu\,\boldsymbol{p},\boldsymbol{q}}^{-,+\,\mathrm{rpa}}(\omega) = \frac{\hbar^2}{|\Lambda|}\left(f_{\mathrm{FD}}(\xi_{\downarrow,\boldsymbol{p}+\boldsymbol{q}})-f_{\mathrm{FD}}(\xi_{\uparrow,\boldsymbol{p}})\right)\left(1-\frac{U}{\hbar^2}\chi_{\beta,\mu\,\boldsymbol{q}}^{-,+\,\mathrm{rpa}}(\omega)\right),\tag{A15a}$$

i.e.,

$$\chi_{\beta,\mu\,\boldsymbol{p},\boldsymbol{q}}^{-,+\,\mathrm{rpa}}(\omega) = \frac{\hbar^2}{|\Lambda|} \frac{f_{\mathrm{FD}}(\xi_{\downarrow,\boldsymbol{p}+\boldsymbol{q}}) - f_{\mathrm{FD}}(\xi_{\uparrow,\boldsymbol{p}})}{\hbar\left(\omega+\mathrm{i}\eta\right) + \xi_{\uparrow,\boldsymbol{p}+\boldsymbol{q}} - \xi_{\downarrow,\boldsymbol{p}}} \left(1 - \frac{U}{\hbar^2} \chi_{\beta,\mu\,\boldsymbol{q}}^{-,+\,\mathrm{rpa}}(\omega)\right). \tag{A15b}$$

Summing over \boldsymbol{p} turns Eq. (A15b) into

$$\chi_{\beta,\mu\,\boldsymbol{q}}^{-,+\,\mathrm{rpa}}(\omega) = -\frac{\Gamma_{\beta,\mu\,\boldsymbol{q}}^{-,+\,\mathrm{rpa}}(\omega)}{1 - \frac{U}{L}\Gamma_{\beta,\mu,\boldsymbol{q}}^{-,+}(\omega)} \tag{A16a}$$

with the definition

$$\Gamma_{\beta,\mu\,\boldsymbol{q}}^{-+}(\omega) := -\frac{\hbar^2}{|\Lambda|} \sum_{\boldsymbol{p}} \frac{f_{\rm FD}(\xi_{\downarrow,\boldsymbol{p}+\boldsymbol{q}}) - f_{\rm FD}(\xi_{\uparrow,\boldsymbol{p}})}{\hbar\,(\omega+\mathrm{i}\eta) + \xi_{\uparrow,\boldsymbol{p}+\boldsymbol{q}} - \xi_{\downarrow,\boldsymbol{p}}},\tag{A16b}$$

and

$$\xi_{\sigma, \boldsymbol{p}} = \xi_{\boldsymbol{p}} + \frac{U}{|\Lambda|} \sum_{\boldsymbol{k} \in \mathrm{BZ}} f_{\mathrm{FD}}(\xi_{\sigma, \boldsymbol{k}}), \qquad \sigma = \uparrow, \downarrow.$$
(A16c)

Equation (5.12) follows after doing the substitutions

$$\boldsymbol{p} = \boldsymbol{k} - \boldsymbol{q}, \qquad \boldsymbol{q} \to -\boldsymbol{q}, \qquad \hbar \to 1,$$
 (A17)

in Eq. (A16).

 N. Nagaosa, Qauntum Field Theory in Strongly Correlated Electronic Systems (Springer-Verlag Berlin Heidelberg 1999).