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Strongly Correlated Systems

prof. Dominik Munzar

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Introduction to magnetic interactions

Dominik Munzar

Department of Condensed Matter Physics, Faculty of Science, Masaryk University

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1. Basic idea and outline

Many magnetic phenomena in solids described using effective Heisenberg-type Hamiltonians.
$H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$,
where J_{ij} are coupling parameters and
$\mathbf{S}_i$ ($\mathbf{S}_j$) is the spin operator connected with the unit i (j).
Unit: orbital, atom, aggregate of atoms etc.
$J_{ij} < 0 / J_{ij} > 0$ ... tendency towards parallel/antiparallel (FM/AF) ordering.
The standard solid state Hamiltonian does not contain any Heisenberg-type terms and the common interaction between magnetic dipoles is too small (see chapter 32 in AM).
What is the origin of these terms?
In this text, the basic strategy for deriving Heisenberg-type Hamiltonians starting from the solid state Hamiltonian will be presented.
Suitable representation of the solid state hamiltonian $\rightarrow$ Neglect of terms that can be assumed not to be important in the given context and/or Construction of an effective Hamiltonian acting on the relevant subspace of the Hilbert space only $\rightarrow$ Transformation of the approximate Hamiltonian into an expression involving Heisenberg-type terms.

2. Description of a many-electron system at the Hartree-Fock level
3. Solid state Hamiltonian in the basis of the Hartree-Fock orbitals and in the basis of the Wannier orbitals
4. Approximations: direct Coulomb repulsions and (simple) exchange terms, the Hunds' rule coupling term
5. Hubbard Hamiltonian
6. Heisenberg Hamiltonian for a simple Mott insulator

2. Description of a many-electron system at the Hartree-Fock level

Solid State Hamiltonian (nuclei fixed):

$$H = \sum_i \left\{ -\frac{\hbar^2}{2m}\nabla_i^2 + v_J(\mathbf{r}_i) \right\} + \frac{1}{2}\sum_{i,j,i\neq j} \frac{e'^2}{|\mathbf{r}_i - \mathbf{r}_j|}\,, v_J(\mathbf{r}) = \sum_J -\frac{Z_J e'^2}{|\mathbf{r} - \mathbf{R}_j|}\,.$$

Hartree-Fock variational ansatz: Slater determinant consisting of Hartree-Fock-Bloch spinorbitals $\varphi_{nk}(\mathbf{r}, \sigma)$.
In this section we consider a non-spin polarized case, i.e., $\varphi_{nk}(\mathbf{r}, \sigma)$ can be written as $\psi_{nk}(\mathbf{r})\chi(\sigma)$, $\chi = \chi_\uparrow$ or $\chi_\downarrow$, ψ does not depend on the spin and the occupation of spin up states is the same as the occupation of spin down states.
Hartree-Fock equation for the Bloch waves:

$$\left\{ -\frac{\hbar^2}{2m}\nabla^2 + v_J(\mathbf{r}) + v_H(\mathbf{r}) + v_x \right\} \psi_{nk}(\mathbf{r}) = \epsilon_{nk}\psi_{nk}(\mathbf{r})\,,$$

where

$$v_H(\mathbf{r}) = 2\sum_{pk',\mathrm{occ.}} \int d\mathbf{r}' \frac{e'^2 |\psi_{pk'}(\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|}\,,$$

$$v_x[\psi] = -\sum_{pk',\mathrm{occ.}} \int d\mathbf{r}' \frac{e'^2 \psi^*_{pk'}(\mathbf{r}')\psi(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \times \psi_{pk'}(\mathbf{r})\,.$$

2. Description of a many-electron system at the Hartree-Fock level

By multiplying both sides of the HF equations by $\psi^*_{nk}(\mathbf{r})$ a integrating $d\mathbf{r}$ we obtain

$$\epsilon_{nk} = \langle n\mathbf{k}|h_1|n\mathbf{k}\rangle + \sum_{pk',\mathrm{occ.}} 2\langle n\mathbf{k}, p\mathbf{k}'\left|\frac{e'^2}{|\Delta\mathbf{r}|}\right|n\mathbf{k}, p\mathbf{k}'\rangle - \sum_{pk',\mathrm{occ.}} \langle n\mathbf{k}, p\mathbf{k}'\left|\frac{e'^2}{|\Delta\mathbf{r}|}\right|p\mathbf{k}', n\mathbf{k}\rangle\,,$$

where

$$h_1 = -\frac{\hbar^2}{2m}\nabla^2 + v_J(\mathbf{r})\,,$$

$$\langle ab\left|\frac{e'^2}{|\Delta\mathbf{r}|}\right|cd\rangle = \int d\mathbf{r}d\mathbf{r}'\frac{e'^2\psi^*_a(\mathbf{r})\psi^*_b(\mathbf{r}')\psi_c(\mathbf{r})\psi_d(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,.$$

The sum of the second and third terms on the right hand side of the equation for ϵ_{nk} will be denoted as $\Delta\varepsilon_{nk}$.

Hartree-Fock based Hamiltonian used in studies of low-energy excited states:

$$H_{H.F.} = \sum_{nks}\varepsilon_{nk}c^\dagger_{nks}c_{nks}\,.$$

3. Solid state H. in the HF basis and in the W. basis, (a) HF

$$H = H_{H.F.} + V_{\rm int} - \Delta H_{HF}\ , \text{ where}$$

$$V_{\rm int} = \frac{1}{2} \sum_{k_1,k_2,k_1',k_2',n,p,q,r,s,s'} \langle n\mathbf{k}_1, p\mathbf{k}_2 \left| \frac{e'^2}{|\Delta \mathbf{r}|} \right| q\mathbf{k}_1', r\mathbf{k}_2' \rangle c^\dagger_{nk_1s} c^\dagger_{pk_2s'} c_{rk_2's'} c_{qk_1's}\ ,$$

and

$$\Delta H_{HF} = \sum_{nks} \Delta\varepsilon_{nk} c^\dagger_{nks} c_{nks} =$$

$$\sum_{nk,pk',s} \left\{ 2\langle n\mathbf{k}, p\mathbf{k}' \left| \frac{e'^2}{|\Delta \mathbf{r}|} \right| n\mathbf{k}, p\mathbf{k}' \rangle - \langle n\mathbf{k}, p\mathbf{k}' \left| \frac{e'^2}{|\Delta \mathbf{r}|} \right| p\mathbf{k}', n\mathbf{k} \rangle \right\} \nu_{pk'} c^\dagger_{nks} c_{nks}\ .$$

Here ν_{pk} is the occupation factor, in the simplest case $\nu_{pk} = 0$ or $\nu_{pk} = 1$. The term ΔH_{HF} has to be subtracted in order to avoid double counting. If the essential effects of the Coulomb interaction are included already at the H.F. level, the term $V_{\rm int} - \Delta H_{HF}$ can be treated as a perturbation. If the interaction term is dominant this is not possible. In such cases it is often more suitable to employ a localized basis set, e.g. the Wannier basis $\{\phi_n(\mathbf{r} - \mathbf{R}_i)\}$. Transformations between the two basis sets:

$$\phi_n(\mathbf{r} - \mathbf{R}_i) = \frac{1}{\sqrt{N}} \sum_k \mathrm{e}^{-i\mathbf{k}\mathbf{R}_i} \psi_{nk}(\mathbf{r})\ , \psi_{nk}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_i \mathrm{e}^{i\mathbf{k}\mathbf{R}_i} \phi_n(\mathbf{r} - \mathbf{R}_i)\ ,$$

$$c_{nks} = \frac{1}{\sqrt{N}} \sum_i \mathrm{e}^{-i\mathbf{k}\mathbf{R}_i} c_{nis}\ ,\ c_{nis} = \frac{1}{\sqrt{N}} \sum_k \mathrm{e}^{i\mathbf{k}\mathbf{R}_i} c_{nks}\ .$$

3. Solid state H. in the HF basis and in the W. basis, (b) W.

Operators $H_{H.F.}$, $V_{\rm int}$, ΔH_{HF}:

$$H_{H.F.} = \sum_{ijns} t_{ijn} c^\dagger_{nis} c_{njs} \; ,$$

where

$$t_{ijn} = \frac{1}{N} \sum_k \varepsilon_{nk} \mathrm{e}^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} \; .$$

$$V_{\rm int} = \frac{1}{2} \sum_{ijkl;npqr;ss'} V(in, jp, kq, lr) c^\dagger_{nis} c^\dagger_{pjs'} c_{rls'} c_{qks} \; ,$$

where

$$V(in, jp, kq, lr) = \int d\mathbf{r} d\mathbf{r}' \frac{e'^2 \phi^*_n(\mathbf{r} - \mathbf{R}_i) \phi^*_p(\mathbf{r}' - \mathbf{R}_j) \phi_q(\mathbf{r} - \mathbf{R}_k) \phi_r(\mathbf{r}' - \mathbf{R}_l)}{|\mathbf{r} - \mathbf{r}'|} \; .$$

$$\Delta H_{HF} = \sum_{ijkl,np,s} \left[2V(in, jp, kn, lp) - V(in, jp, lp, kn) \right] \nu_{jlp} c^\dagger_{nis} c_{nks} \; ,$$

where

$$\nu_{jlp} = \frac{1}{N} \sum_k \nu_{pk} \mathrm{e}^{i\mathbf{k}(\mathbf{R}_j - \mathbf{R}_l)} \; .$$

4. Approximations: direct Coulomb repulsions and exchange terms ...

The expression for V_{int} on the previous slide is fairly complicated. For this reason, usually only two classes of coupling terms are taken into account.
(a) Direct Coulomb repulsions, i.e., terms with $(in) = (kq)$ a $(jp) = (lr)$;
(b) Exchange terms, i.e., terms with $(in) = (lr)$ a $(jp) = (kq)$.
Ad (a).

$$V_{\mathrm{c}} = \frac{1}{2} \sum_{ij,np,ss',(ins)\neq(jps')} V_{ijnp} n_{nis} n_{pjs'} \, ,$$

where

$$V_{ijnp} = \int d\mathbf{r} d\mathbf{r}' \frac{e'^2 |\phi_n(\mathbf{r}-\mathbf{R}_i)|^2 \, |\phi_p(\mathbf{r}'-\mathbf{R}_j)|^2}{|\mathbf{r}-\mathbf{r}'|}$$

is the so called Coulomb integral and $n_{nis} = c^\dagger_{nis} c_{nis}$. For a single band (n), i.e., just one W. orbital per atom, we obtain the Hubbard interaction term:

$$V_{\mathrm{c}} = \sum_i U n_{ni\uparrow} n_{ni\downarrow}$$

with $V_{ijnn} = \delta_{ij} U$.

4. Approximations: direct Coulomb repulsions and exchange terms ...

Ad (b).

$$V_{\text{ex}} = \frac{1}{2} \sum_{ijnp, in \neq jp, ss'} J_{ijnp} c^\dagger_{nis} c^\dagger_{pjs'} c_{nis'} c_{pjs} \, ,$$

where

$$J_{ijnp} = \int d\mathbf{r} d\mathbf{r}' \frac{e'^2 \phi_n^*(\mathbf{r} - \mathbf{R}_i) \phi_p^*(\mathbf{r}' - \mathbf{R}_j) \phi_p(\mathbf{r} - \mathbf{R}_j) \phi_n(\mathbf{r}' - \mathbf{R}_i)}{|\mathbf{r} - \mathbf{r}'|}$$

is the so called exchange integral. The term with $in = jp$ is excluded because it is contained already in the direct Coulomb term. The expressiom for V_{ex} can be simplified by introducing spin operators $\mathbf{S}_{in} = (S^x_{in}, S^y_{in}, S^z_{in})$:

$$S^{x/y/z}_{in} = \frac{1}{2} (c^+_{in\uparrow}, c^+_{in\downarrow}) \Big(\sigma_{x/y/z} \Big) \begin{pmatrix} c_{in\uparrow} \\ c_{in\downarrow} \end{pmatrix} \, , \sigma_x = \begin{pmatrix} 0 1 \\ 1 0 \end{pmatrix} \, , \sigma_y = \begin{pmatrix} 0 - i \\ i \ 0 \end{pmatrix} \, , \sigma_z = \begin{pmatrix} 1 \ 0 \\ 0 - 1 \end{pmatrix} \, .$$

Physical meaning of $\mathbf{S}_{in}$: it is a one particle operator, that can be expressed as $\sum_k \mathbf{s}_k P_{k,in}$, with the sum running over all electrons, $\mathbf{s}_k$ is the spin operator of the k-th electron (in units of $\hbar$) and $P_{k,in}$ is the projector on the subspace corresponding to the W. orbital $\phi_n(\mathbf{r} - \mathbf{R}_i)$. After some manipulations we obtain

$$V_{\text{ex}} = - \sum_{ijnp, in \neq jp} J_{ijnp} [\mathbf{S}_{in} \cdot \mathbf{S}_{jp} + \frac{1}{4} n_{in} n_{jp}] \, .$$

4. Approximations: Discussion of the exchange term

$$V_{\rm ex} = - \sum_{ijnp, in \neq jp} J_{ijnp} [\mathbf{S}_{in} \cdot \mathbf{S}_{jp} + \frac{1}{4} n_{in} n_{jp}] \, .$$

Remarks:
(i) In some cases, the occupations of the Wannier orbitals can be assumed to be fixed, the operators n_{in} a n_{ip} can then be replaced with their eigenvalues and only spin degrees of freedom remain active. In the following considerations we assume that this is the case.
(ii) J_{ijnp} is a positive real number. $V_{\rm ex}$ thus prefers configurations with parallel spins (FM).
(iii) Interpretation: electrons with parallel spins avoid each other better than electrons with antiparallel spins, a consequence of the Pauli principle.
(iv) J_{ijnp} decreases approximately exponentially with increasing distance $|\mathbf{R}_i - \mathbf{R}_j|$. The elements J_{iinp} are therefore much larger than elements with $j \neq i$, and the latter can be usually neglected. We obtain

$$V_{\rm ex} \approx - \sum_{inp, n \neq p} J_{iinp} \mathbf{S}_{in} \cdot \mathbf{S}_{ip} \, .$$

The term containing n_{in} a n_{jp} has been omitted. The formula allows us to interpret the first Hund's rule, the expression on the r. h. s. is therefore labelled as the H. rule coupling term.
(v) The latter plays an essential role in the theory of ferromagnetism, but it is not the only player. Realistic models include, in addition, the one-particle term (the effective kinetic energy) and the on-site Coulomb repulsions. A description of a common ferromagnet in terms of a Heisenberg-type Hamiltonian is a phenomenological one.

5. Hubbard Hamiltonian

Here we address the one-band Hamiltonian with the Hubbard interaction term, the so called Hubbard Hamiltonian:

$$H = \sum_{ijs} t_{ij} c_{is}^\dagger c_{js} + \sum_i U n_{i\uparrow} n_{i\downarrow} \,.$$

The band index has been omitted for simplicity.

(a) Physical interpretation of the first term.
Consider the case of $|\Psi(0)\rangle = c_j^\dagger |0\rangle$. Using the Schrödinger equation we obtain

$$|\Psi(t)\rangle = c_j^\dagger |0\rangle - \frac{it}{\hbar} \sum_i t_{ij} c_i^\dagger |0\rangle$$

for sufficiently small values of t. The amplitude of the transition ("hopping") from j do i per unit time is thus $-(i/\hbar) t_{ij}$.
t_{ij} ... "hopping matrix element"
$\sum_{ijs} t_{ij} c_{is}^\dagger c_{js}$ ... "hopping term", "effective kinetic energy"

(b) Physical interpretation of the second term.
On-site Coulomb repulsions between electrons with antiparallel spins. The term is used to describe correlations between spin up and spin down electrons, that are not included in the H. F. theory. ,,Effective potential energy".

5. Hubbard Hamiltonian, estimates of U ...

(c) Estimates of U and of some other matrix elements.
Consider $3d$ orbitals of an atom of a 4th-period transition metal.
Rough estimate of the expectation value of the interaction between the nucleus and a $3d$ electron:

$$\langle V \rangle \approx -\frac{2Z^{*2}\mathrm{Ry}}{n^2}\,,$$

where Z^* is the effective charge of the nucleus, $Z^* \approx 5-10$, and $n = 3$. We obtain $\langle V \rangle \approx 50 - 200\,\mathrm{eV}$.

Rough estimate of U:

$$U \approx \frac{2Z^*\mathrm{Ry}}{n^2} \approx 15 - 30\,\mathrm{eV}\,.$$

It can be seen that the values of U are comparable with the conduction band bandwith of the order of tens of eV.

Rough estimate of matrix elements of the type $\langle i,j \left| \frac{e'^2}{|\Delta \mathbf{r}|} \right| i,j \rangle$, where i,j are nearest neighbours. For the sake of simplicity, let us assume that the Wannier orbital are fairly localized. Then we have

$$\langle i,j \left| \frac{e'^2}{|\Delta \mathbf{r}|} \right| i,j \rangle \approx \frac{2\mathrm{Ry}}{R[a_0]}\,,$$

where R is the distance between nearest neighbours. For transition metals we have $R \approx 5a_0$ and $\langle i,j \left| \frac{e'^2}{|\Delta \mathbf{r}|} \right| i,j \rangle \approx 5\,\mathrm{eV}$. The Coulomb interaction between two electrons at i or between an electron at i and an electron at j will be further reduced by screening effects.

5. Hubbard Hamiltonian, estimates of U ...

Rough estimate of matrix elements of the type $\langle i,i \left| \frac{e'^2}{|\Delta \mathbf{r}|} \right| i,j \rangle$, with i,j nearest neighbours.

$$\langle i,i \left| \frac{e'^2}{|\Delta \mathbf{r}|} \right| i,j \rangle = \int d\mathbf{r} d\mathbf{r}' \frac{e'^2 \phi^*(\mathbf{r}-\mathbf{R}_i)\phi^*(\mathbf{r}'-\mathbf{R}_i)\phi(\mathbf{r}-\mathbf{R}_i)\phi(\mathbf{r}'-\mathbf{R}_j)}{|\mathbf{r}-\mathbf{r}'|} \, .$$

This expression can be viewed as the interaction energy of a charge cloud of the density $e\phi^*(\mathbf{r}-\mathbf{R}_i)\phi(\mathbf{r}-\mathbf{R}_i)$ and a charge cloud of the density $e\phi^*(\mathbf{r}-\mathbf{R}_i)\phi(\mathbf{r}-\mathbf{R}_j)$, the so called overlap charge density. The absolute value of the overlap charge q is approximately by an order of magnitude lower than $|e|$. Therefore

$$\langle i,i \left| \frac{e'^2}{|\Delta \mathbf{r}|} \right| i,j \rangle \approx \frac{2q\mathrm{Ry}}{0.5R[a_0]} \approx 1\,\mathrm{eV} \, .$$

The above estimates allow us to conclude that the matrix element U is indeed considerably larger than other Coulomb interaction matrix elements and that it is likely to play the main role in the physics of local electronic correlations.

5. Hubbard Hamiltonian, general remarks

(d) General remarks on the Hubbard Hamiltonian

- It is the simplest possible Hamiltonian allowing one to address correlations between spin up and spin down electrons.

- Fundamental role in theory of magnetism and superconductivity.

- Analytical solutions only in the 1D case and in the ∞D case, for a basic information, see chapter 12.5.3 in Fulde's textbook.

- Effective kinetic energy (T in the following) and the effective potential energy (V_H in the following) play here similar roles as the kinetic energy and the potential energy in one-particle quantum mechanics (delocalizing electrons and localizing electrons, respectively).

5. Hubbard Hamiltonian, limiting cases

(e) Limiting cases.
(α) First limiting case: $U = 0$.
(β) Second limiting case: $t = 0$.
Ad (α). This is the so called "band limit". Exact solution: Slater determinant consisting of H. F. B. states.
In the following (including part (β)), for concreteness, we consider a simple one-dimensional lattice with lattice parameter a, N lattice points and N electrons. One-particle states: $\psi_k \chi_\uparrow$, $\psi_k \chi_\downarrow$, energies: $\varepsilon_k = 2t\cos(ka)$, quasiparticle operators: c_{ks}, $c^\dagger_{ks}$.
The ground state is nondegenerate,

$$|\Psi_\alpha\rangle = \Pi_{-\frac{\pi}{2a}<k<\frac{\pi}{2a}} c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} |0\rangle \, .$$

Ad (β). This is the so called "atomic limit". In the ground state, there is one electron at each lattice site - this minimizes the effective potential energy. The charge distribution is thus given, the spin distribution, however, may be arbitrary, and the ground state is 2^N degenerate,

$$|\Psi_\beta\rangle = \Pi_{i=1}^N c^\dagger_{i\uparrow} / c^\dagger_{i\downarrow} |0\rangle \, .$$

5. Hubbard Hamiltonian, Mott transition

(f) Mott transition.

$$|\Psi_\alpha\rangle = \Pi_{-\frac{\pi}{2a}<k<\frac{\pi}{2a}} c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} |0\rangle \;, \; |\Psi_\beta\rangle = \Pi_{i=1}^N c^\dagger_{i\uparrow}/c^\dagger_{i\downarrow}|0\rangle$$

For finite U and t none of the state vectors $|\Psi_\alpha\rangle$, $|\Psi_\beta\rangle$ is an eigenvector. We can, however, pose the following question: Which of the two vectors provides a better description of the ground state (i.e., a lower value of $\langle H \rangle$)? We obtain

$$\langle\Psi_\alpha|T|\Psi_\alpha\rangle = \frac{4tN}{\pi}\,,\; \langle\Psi_\alpha|V_H|\Psi_\alpha\rangle = \frac{NU}{4}\,,\; \langle\Psi_\alpha|H|\Psi_\alpha\rangle = \frac{4tN}{\pi} + \frac{NU}{4}\,.$$

$$\langle\Psi_\beta|T|\Psi_\beta\rangle = 0\,,\; \langle\Psi_\beta|V_H|\Psi_\beta\rangle = 0\,,\; \langle\Psi_\beta|H|\Psi_\beta\rangle = 0\,.$$

Clearly, for $U < 16|t|/\pi$ ($U > 16|t|/\pi$), the state vector $|\Psi_\alpha\rangle$ (any of the state vectors $|\Psi_\beta\rangle$) represents a better variational ansatz. Recall that $t < 0$ (remember the corresponding description of the hydrogen molecule) and that $16|t|/\pi$ is very approximately equal to the bandwidth $W = 4|t|$. Results of more sophisticated calculations demonstrate that

for $W > U$ the electrons are delocalized and the system behaves as a metal, in agreement with the rule that an odd number of electrons per unit cell implies a metallic behaviour,

for $W < U$ the electrons are localized and the system behaves as an insulator, the so called Mott insulator, in contrast with the above mentioned rule.

This is the so called Mott criterion and the transition between the metallic state and the insulating state is denoted as the Mott transition. The essential property of the Mott insulator is that the charge degrees of freedom are frozen and only the spins remain "alive".

6. Heisenberg Hamiltonian for a simple Mott insulator

In order to derive an effective spin Hamiltonian, we consider first, for the sake of simplicity, the case of $N = 2$, we have two sites and two electrons. The Hubbard Hamiltonian reads

$$H = T + V_H \, , \, T = \sum_s t(c^\dagger_{2s} c_{1s} + c^\dagger_{1s} c_{2s}) \, , \, V_H = U n_{1\uparrow} n_{1\downarrow} + U n_{2\uparrow} n_{2\downarrow} \, .$$

We shall limit ourselves to the case of $U >> t$. The interaction term (i.e., the Hamiltonian of the atomic limit) can be considered as the "unperturbed" Hamiltonian and the kinetic energy term as a perturbation. Solutions of the unperturbed problem are

$$|\uparrow|\uparrow\rangle \, , \, |\uparrow|\downarrow\rangle \, , \, |\downarrow|\uparrow\rangle \, , \, |\downarrow|\downarrow\rangle \ldots E = 0 \text{ subspace } L$$

$$|\uparrow\downarrow|-\rangle \, , \, |-|\uparrow\downarrow\rangle \ldots E = U \text{ subspace } H \, .$$

Next we focus on state vectors thats evolve, "after the application of the perturbation", from the low-energy subspace L. Our aim is to find an effective Hamiltonian H_{ef} acting on L such that, *if* $|\Psi\rangle$ *satisfies* $H|\Psi\rangle = E|\Psi\rangle$, $H_{ef} P_L |\Psi\rangle = E P_L |\Psi\rangle$.
Here P_L is the projector on the subspace L.

Assume thus that $|\Psi\rangle$ satisfies $H|\Psi\rangle = E|\Psi\rangle$. The Hamiltonian can be expressed in terms of the projection operators:

$$H = P_L H P_L + P_L H P_H + P_H H P_L + P_H H P_H = P_L V_H P_L + P_H V_H P_H + P_H T P_L + P_L T P_H$$

and $|\Psi\rangle = |\Psi_L\rangle + |\Psi_H\rangle$, where $|\Psi_L\rangle = P_L|\Psi\rangle$ and $|\Psi_H\rangle = P_H|\Psi\rangle$. After inserting this into Eq. $H|\Psi\rangle = E|\Psi\rangle$ we obtain

6. Heisenberg Hamiltonian for a simple Mott insulator

$$(P_L V_H P_L + P_H V_H P_H + P_H T P_L + P_L T P_H)(|\Psi_L\rangle + |\Psi_H\rangle) = E(|\Psi_L\rangle + |\Psi_H\rangle) .$$

Let us act on this equation first with P_L and second with P_H. We obtain:

$$P_L V_H P_L|\Psi_L\rangle + P_L T P_H|\Psi_H\rangle = E|\Psi_L\rangle ,$$

$$P_H V_H P_H|\Psi_H\rangle + P_H T P_L|\Psi_L\rangle = E|\Psi_H\rangle .$$

We use the second equation to express $|\Psi_H\rangle$,

$$|\Psi_H\rangle = \frac{1}{E - P_H V_H P_H} P_H T P_L|\Psi_L\rangle ,$$

and insert this into the first equation. We obtain

$$\left\{ P_L V_H P_L + P_L T P_H \frac{1}{E - P_H V_H P_H} P_H T P_L \right\} |\Psi_L\rangle = E|\Psi_L\rangle .$$

Using $P_L V_H P_L = 0$ a $P_H V_H P_H = P_H U P_H$ we further obtain

$$\frac{P_L T P_H T P_L}{E - U}|\Psi_L\rangle = E|\Psi_L\rangle .$$

The last equation is still, within the given model, exact. For $E << U$ (applies to the low energy sector), we can neglect E as compared to U in the denominator and we obtain

$$H_{ef}|\Psi_L\rangle = E|\Psi_L\rangle \text{ with } H_{ef} = -\frac{P_L T P_H T P_L}{U} .$$

6. Heisenberg Hamiltonian for a simple Mott insulator

Next we express H_{ef} in terms of spin operators. Using explicit representations of the projectors P_L and P_H we obtain

$$H_{ef} = -\frac{1}{U} \sum_{i,j,i \in L, j \in L} |i\rangle\langle i| T \left[\sum_{k \in H} |k\rangle\langle k| \right] T |j\rangle\langle j| \,. \qquad (2)$$

Using $\sum_{k \in H} = 1 - \sum_{k \in L}$ and the fact that matrix elements of T on the subspace L are equal to zero we further obtain

$$H_{ef} = -\frac{P_L T^2 P_L}{U} = -\frac{1}{U} P_L \left[\sum_s t(c^\dagger_{2s} c_{1s} + c^\dagger_{1s} c_{2s}) \right]^2 P_L =$$

$$= P_L J \left(\mathbf{S}_1 \cdot \mathbf{S}_2 - \frac{n_1 n_2}{4} \right) P_L \,,$$

where $J = 4t^2/U$. In the final expression, the symbols P_L are usually omitted.

In a more general case of N lattice sites and N electrons we obtain

$$H_{ef} = \frac{1}{2} P_L \sum_{i,j,i \neq j} J_{ij} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right) P_L \,,$$

where $J_{ij} = 4t^2_{ij}/U$. Again, the symbols P_L are usually omitted.

6. Heisenberg Hamiltonian for a simple Mott insulator

Concluding remarks:

(i) As in the case of the spin representation of $V_{\rm ex}$, it is not necessary to consider the $n_i n_j$ term of the effective Hamiltonian, in conjunction with the projectors, it provides a constant contribution.

(ii) The interaction constants J_{ij} are positive, the (ij) term therefore prefers configurations with antiparallel spins at sites i a j (AF).

(iii) Interpretation. For simplicity, consider $N = 2$. In a configuration with parallel spins, none of the electrons can hop to the neighbouring site, this is not allowed by the Pauli principle. In a configuration with antiparallel spins, any electron can "visit" the neighbouring site. This is not blocked by the Pauli principle. Of course, the electrons are still localized by U, but the probabilities of the visits are finite. It implies that configurations with antiparallel spins exhibit a lower kinetic energy than those with parallels spins. The mechanism is therefore labelled as "**kinetic exchange**" . In real Mott insulators the hoppings proceed via intermediate atoms and the mechanism is labelled as "**superexchange interaction**".

More rigorously: matrix elements of T between states of the subspace L and states of the subspace H are nonzero. Degenerate perturbation theory provides the corresponding effective interaction on L.

(iv) The values of the interaction constants J_{ij} can be in principle obtained by first principles calculations.

Dynamical Mean Field Theory

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I. INTRODUCTION

The Dynamical Mean Field Theory (DMFT) is a technique whose development relied on the essential contributions by Metzner and Vollhardt[1], Metzner[2], Müller-Hartmann[3], Georges and Kotliar[4], and Jarrell[5]. DMFT has been developing rapidly since the first days of its introduction, and many reference articles, reviews and PhD thesis are available[2,6–10]. The derivation we present here is called the "cavity" method, after an approach extensively used in classical statistical mechanics. Georges and collaborators applied its concepts to the derivation of the DMFT equations[11]. This is by no means the only possible way to proceed, but has the advantage of providing a straightforward physical interpretation of the approach, and also of highlighting the links between the DMFT approach and other well-known mean field theories. Another popular approach is based on the expansion of the free energy and the correlation functions around the atomic limit. The latter was initiated by the pioneering work of Metzner and Vollhardt[1], who demonstrated the simplifications brought about by the $d \to \infty$ limit applied to the Hubbard model.

DMFT is a mean-field theory, and can be viewed as an extension of the well known mean field approach applied to the Ising model. For example, the mean-field approximation of the Ising model becomes exact in the limit of infinite coordination, and the same is true for DMFT. Intuitively, this can be understood because in the limit of infinite coordination, the neighbors of a given site are seen, from this site, as a continuous "bath", which indeed corresponds to a mean-field.

In the cavity method, a particular site of the lattice is singled out, e.g., site o, indexed by $i = 0$. The degrees of freedom of all the other sites are then integrated out, which allows the derivation of an effective Hamiltonian for site o. This Hamiltonian may be mapped onto a single-impurity Anderson model. The comparison is most easily expressed in the functional integral representation of these effective models. Thus, we first illustrate the way the non-desired degrees of freedom are integrated out in the framework of the Lagrangian representation of the physics of a few models. We first examine the case of a non interacting system, in order to identify how the Green's function is present inside the Lagrangian formulation. Then, we derive effective models for the single impurity Anderson model and the Hubbard model in the limit of infinite coordination, and demonstrate how they are related. This will allow us to develop a system of self-consistent equations, which can be iterated to find the solution of the problem at hand, provided the impurity problem can be solved. The numerical approach to the solution of the impurity problem is an active research topic in itself.

II. COHERENT STATES FOR FERMIONS

The simplest possible mean-field approach to the Hubbard model is based on the assumption that the fluctuations of the density of electrons on a site are small compared to the value of the average. This allows the interaction term to be transformed from a quartic form to a quadratic form, and provides some useful insights into the physics of the model. A deeper insight can be gained in a more natural and concise way by using the path-integral formalism, which we will now introduce. Once this formalism is introduced, we will use it to derive an alternative mean-field approach to the one-band Hubbard model, which will provide the so-called spin-fermion model. The material in this section follows closely the derivations provided in Ref.[12]

A. The basis of coherent states

When dealing with many-body fermionic systems, it is frequent to make use of Slater determinants in order to obtain a set of suitably symmetrized states forming a basis of the Fock space. Another extremely useful basis of the Fock space is the basis of coherent states[12]. Although it is not an orthonormal basis, it spans the whole Fock space. Just as the states $|\boldsymbol{r}\rangle$ are defined as eigenstates of the position operator $\hat{\boldsymbol{r}}$, the coherent states are defined as eigenstates of the annihilation operators. It is instructive to examine why annihilation operators, rather than creation operators, are considered for this purpose. Let us consider a general vector of the Fock space $|\phi\rangle$ and expand it in the occupation number basis:

$$|\phi\rangle = \sum_{n=0}^{\infty} \sum_{\alpha_1 \ldots \alpha_n} \phi_{\alpha_1 \alpha_n} \left|\alpha_1 \ldots \alpha_n\right\rangle , \qquad (1)$$

where $|\alpha_1 \ldots \alpha_n\rangle$ is a many-particle state where single-particle states $\alpha_1, \ldots \alpha_n$ are occupied. Now, consider the infinite but countable set made up of the positive numbers of particles in each of the components of $|\phi\rangle$. This set being countable, made up of integer numbers greater than or equal to 0, it possesses a smallest element. Application of a creation operator increases the value of this smallest element in the obtained ket by one, and therefore the image ket cannot be a multiple of $|\phi\rangle$: a creation operator cannot have an eigenstate. On the other hand, this set does not necessarily possess a largest element: physically, $|\phi\rangle$ may contain components with all particle numbers. As a consequence, application of an annihilation operator does not preclude the image ket to be proportional to $|\phi\rangle$. In other terms, nothing forbids the ket $|\phi\rangle$ to be an eigenstate.

Assuming such an eigenstate $|\phi\rangle$ of the annihilation operators a_α has been found, then

$$a_\alpha |\phi\rangle = \phi_\alpha |\phi\rangle .$$

The commutation (anticommutation) relations of the creation and annihilation operators for bosons (fermions) then have an interesting consequence for the eigenvalues ϕ_α. For bosons, the eigenvalues commute, and can therefore be ordinary complex numbers. For fermions though, the eigenvalues anticommute, $\phi_\beta\phi_\alpha = -\phi_\alpha\phi_\beta$. This requires the introduction of anticommuting variables, called Grassmann numbers, which we will now focus on.

B. Grassmann algebra

Algebras of anticommuting numbers are called Grassmann algebras. For our purpose, it will be sufficient to view the rules of Grassmann algebra as a clever mathematical construct, which takes care of all the minus signs related to the necessary symmetrization of fermionic states, in the same way as second quantization does it. For a more thorough mathematical treatment of these algebras, we refer the reader to Ref.[13]. A Grassmann algebra is defined by a set of generators $\{\xi_\alpha\}$, $\alpha = 1, \ldots, n$. Such generators anticommute, $\xi_\beta\xi_\alpha + \xi_\alpha\xi_\beta = 0$, so that $\xi_\alpha^2 = 0$. The set of all distinct products of the generators makes up a basis of the algebra: any number in the Grassmann algebra is a linear combination with complex coefficients of the numbers from the set $\{1, \xi_{\alpha_1}, \ldots, \xi_{\alpha_1}\xi_{\alpha_2}, \ldots, \xi_{\alpha_1}\xi_{\alpha_2}\ldots\xi_{\alpha_n}\}$ where by convention the indices are ordered: $\alpha_1 < \alpha_2 < \ldots < \alpha_n$. The dimension of the algebra is therefore 2^n.

In an algebra with an even set $n = 2p$ of generators, conjugation is defined as follows: a set of p generators is selected, and to each of these ξ_α, a different generator among the other p is associated, and denoted ξ_α^*. The following properties then define conjugation in the Grassmann algebra:

$$(\xi_\alpha)^* = \xi^*_\alpha$$
$$(\xi^*_\alpha)^* = \xi_\alpha$$
$$\forall \lambda \in \mathbb{C},\ (\lambda \xi_\alpha)^* = \lambda^* \xi^*_\alpha$$
$$(\xi_{\alpha_1}\xi_{\alpha_2}\dots\xi_{\alpha_n})^* = \xi^*_{\alpha_n}\dots\xi^*_{\alpha_2}\xi^*_{\alpha_1}.$$

In the following, we focus for clarity on a Grassmann algebra possessing two generators. As a consequence of $\xi^2 = 0$, we find that any analytic function f on this algebra is a linear function, and that a function A of two Grassmann variables ξ and ξ^* has the following form:

$$f(\xi) = f_0 + f_1\xi$$
$$A(\xi, \xi^*) = a_0 + a_1\xi + \overline{a_1}\xi^* + a_{12}\xi^*\xi.$$

Note that a_1 and $\overline{a_1}$ are not necessarily complex conjugates of each other.

A derivative on these functions may be defined, as it is for ordinary complex functions, only in this case, the variable ξ has to be anticommuted through, until adjacent to the relevant $\dfrac{\partial}{\partial \xi}$, e.g.:

$$\frac{\partial}{\partial \xi}(\xi^*\xi) = -\frac{\partial}{\partial \xi}(\xi\xi^*) = -\xi^*.$$

Note that with this definition, the operators $\dfrac{\partial}{\partial \xi}$ and $\dfrac{\partial}{\partial \xi^*}$ anticommute.

For integration, there is no analog to the familiar Riemann integral construction for ordinary variables. Instead, integration over Grassmann variables is defined as a linear mapping which respects the fundamental property that the integral of an exact differential form is zero. With this, considering that 1 is the derivative of ξ, while ξ is not a derivative, we find the following rules, which define integration:

$$\int d\xi \xi = 1$$
$$\int d\xi 1 = 0.$$

Note that in these expressions, $d\xi$ does not represent an infinitesimal Grassmann number, but is only a notational convenience, and that an expression such as $\int d\xi^*\xi$ does not make sense. A convenient way to remember these definitions is to remark that integration and differentiation are identical on the Grassmann algebra.

Finally, we may equip the space of functions over the Grassmann algebra with a scalar product, e.g. for $f \equiv f_0 + f_1\xi$ and $g(\xi) \equiv g_0 + g_1\xi$:

$$\begin{aligned}\langle f|g\rangle &\equiv \int d\xi^*\, d\xi\, e^{-\xi^*\xi}\, f^*(\xi)\, g(\xi^*) \\ &= \int d\xi^*\, d\xi\, (1-\xi^*\,\xi)(f_0^* + f_1^*\xi)(g_0 + g_1\xi^*) \\ &= -\int d\xi^*\, d\xi\, \xi^*\,\xi f_0^* g_0 + \int d\xi^*\, d\xi\, \xi\, \xi^*\, f_1^* g_1 \\ &= f_0^* g_0 + f_1^* g_1.\end{aligned}$$

It can be shown that with this definition of the product, functions of Grassmann variables form a Hilbert space.

C. Coherent states for fermionic systems

In this section, we will give an explicit expression for the fermion coherent states. As illustrated above, any relevant expansion – of the kind Eq. (1) – must involve Grassmann numbers as coefficients. Therefore, any attempt at an expression for the fermion coherent states requires that the Fock space be enlarged. To this end, a Grassmann algebra $\mathcal{G}$ is defined, by associating a generator ξ_α (ξ_α^*) to each annihilation (creation) operator a_α ($a_\alpha^\dagger$). The generalized Fock space is then constructed as the set of linear combinations of elements of the Fock space $\mathcal{F}$, with coefficients in the Grassmann algebra $\mathcal{G}$:

$$|\psi\rangle = \sum_\alpha \chi_\alpha \,|\phi_\alpha\rangle\,,$$

where $\chi_\alpha \in \mathcal{G}$, and $|\phi_\alpha\rangle \in \mathcal{F}$. Finally, we require the following relations between elements of $\mathcal{G}$ and the creation/annihilation operators:

$$\begin{aligned}\left[\tilde{\xi}, \tilde{a}\right]_+ &= 0 \\ \left(\tilde{\xi}\tilde{a}\right)^\dagger &= \tilde{a}^\dagger \tilde{\xi}^*,\end{aligned}$$

where $\tilde{\xi}$ is any Grassmann variable in $\{\xi_\alpha, \xi_\alpha^*\}$, and $\tilde{a}$ any operator in $\left\{a_\alpha, a_\alpha^\dagger\right\}$.

We are now in a position to introduce the fermion coherent state (this definition closely follows that used in the bosonic case):

$$|\xi\rangle = e^{-\sum_\alpha \xi_\alpha a_\alpha^\dagger}\,|0\rangle = \prod_\alpha \left(1 - \xi_\alpha a_\alpha^\dagger\right)|0\rangle\,,$$

where we have used the fact that $\xi_\alpha a^\dagger_\alpha$ and $\xi_\beta a^\dagger_\beta$ commute. For any state α, we have

$$\begin{aligned} a_\alpha\big(1-\xi_\alpha a^\dagger_\alpha\big)\left|0\right\rangle = \xi_\alpha\left|0\right\rangle &= \xi_\alpha\big(1-\xi_\alpha a^\dagger_\alpha\big)\left|0\right\rangle \\ \Rightarrow a_\alpha\left|\xi\right\rangle &= \prod_{\beta\neq\alpha}\Big(1-\xi_\beta a^\dagger_\beta\Big)a_\alpha\big(1-\xi_\alpha a^\dagger_\alpha\big)\left|0\right\rangle \\ &= \prod_{\beta\neq\alpha}\Big(1-\xi_\beta a^\dagger_\beta\Big)\xi_\alpha\big(1-\xi_\alpha a^\dagger_\alpha\big)\left|0\right\rangle \\ &= \xi_\alpha\prod_{\beta}\Big(1-\xi_\beta a^\dagger_\beta\Big)\left|0\right\rangle = \xi_\alpha\left|\xi\right\rangle . \end{aligned} \tag{2}$$

The action of $a^\dagger_\alpha$ on a coherent state is as follows:

$$\begin{aligned} a^\dagger_\alpha\left|\xi\right\rangle &= a^\dagger_\alpha\big(1-\xi_\alpha a^\dagger_\alpha\big)\prod_{\beta\neq\alpha}\Big(1-\xi_\beta a^\dagger_\beta\Big)\left|0\right\rangle \\ &= a^\dagger_\alpha\prod_{\beta\neq\alpha}\Big(1-\xi_\beta a^\dagger_\beta\Big)\left|0\right\rangle \\ &= -\frac{\partial}{\partial\xi_\alpha}\big(1-\xi_\alpha a^\dagger_\alpha\big)\prod_{\beta\neq\alpha}\Big(1-\xi_\beta a^\dagger_\beta\Big)\left|0\right\rangle = -\frac{\partial}{\partial\xi_\alpha}\left|\xi\right\rangle \end{aligned}$$

Similarly, the adjoint of the coherent state is

$$\left\langle\xi\right| = \left\langle 0\right| e^{-\sum_\alpha a_\alpha\xi^*_\alpha} = \left\langle 0\right| e^{\sum_\alpha \xi^*_\alpha a_\alpha},$$

with $\left\langle\xi\right| a^\dagger_\alpha = \left\langle\xi\right|\xi^*_\alpha$, and one can verify that

$$\left\langle\xi\right| a_\alpha = \frac{\partial}{\partial\xi^*_\alpha}\left\langle\xi\right| . \tag{3}$$

D. Algebraic properties of the fermion coherent state basis

The overlap between coherent states is given by:

$$\begin{aligned} \left\langle\xi|\xi'\right\rangle &= \left\langle 0\right|\prod_\alpha\left(1+\xi^*_\alpha a_\alpha\right)\prod_\beta\Big(1-\xi'_\beta a^\dagger_\beta\Big)\left|0\right\rangle \\ &= \left\langle 0\right|\prod_{\alpha,\beta}\left(1+\xi^*_\alpha a_\alpha\right)\Big(1-\xi'_\beta a^\dagger_\beta\Big)\left|0\right\rangle \\ &= \prod_\alpha\left(1+\xi^*_\alpha\xi'_\alpha\right) \\ &= e^{\sum_\alpha\xi^*_\alpha\xi'_\alpha}, \end{aligned} \tag{4}$$

which shows that coherent states are not orthogonal.

Whenever dealing with (over)complete basis of the Fock space, the closure relation is an essential ingredient. We will now establish its form for coherent states. Let us define the operator

$$A = \int \prod_\alpha d\xi^*_\alpha \, d\xi_\alpha \, e^{-\sum_\alpha \xi^*_\alpha \xi_\alpha} \, |\xi\rangle\langle\xi| \, .$$

Using the eigenvalue property of the coherent states, we have

$$\begin{aligned} \langle \alpha_1 \ldots \alpha_n | \xi \rangle &= \langle 0 | a_{\alpha_1} \ldots a_{\alpha_n} | \xi \rangle \\ &= \langle 0 | \xi_{\alpha_1} \ldots \xi_{\alpha_n} | \xi \rangle \\ &= \langle 0 | \xi_{\alpha_1} \ldots \xi_{\alpha_n} \prod_\alpha \left(1 - \xi_\alpha a^\dagger_\alpha\right) | 0 \rangle \\ &= \xi_{\alpha_1} \ldots \xi_{\alpha_n} , \end{aligned}$$

and the similar adjoint equation. Thus, for any vectors $|\alpha_1 \ldots \alpha_n\rangle$ and $|\beta_1 \ldots \beta_m\rangle$ of the basis of the Fock space,

$$\begin{aligned} \langle \alpha_1 \ldots \alpha_n | A | \beta_1 \ldots \beta_m \rangle &= \int \prod_\alpha d\xi^*_\alpha \, d\xi_\alpha e^{-\sum_\alpha \xi^*_\alpha \xi_\alpha} \langle \alpha_1 \ldots \alpha_n | \xi \rangle \, \langle \xi | \beta_1 \ldots \beta_m \rangle \\ &= \int \prod_\alpha d\xi^*_\alpha \, d\xi_\alpha \prod_\alpha (1 - \xi^*_\alpha \, \xi_\alpha) \xi_{\alpha_1} \ldots \xi_{\alpha_n} \xi^*_{\beta_1} \ldots \xi^*_{\beta_m} . \end{aligned} \tag{5}$$

We can now consider the kinds of integrals which may appear, for a specific state γ:

$$\int d\xi^*_\gamma \, d\xi_\gamma \left(1 - \xi^*_\gamma \, \xi_\gamma\right) \left\{ \begin{array}{c} \xi_\gamma \, \xi^*_\gamma \\ \xi_\gamma \\ \xi^*_\gamma \\ 1 \end{array} \right\} = \left\{ \begin{array}{c} 1 \\ 0 \\ 0 \\ 1 \end{array} \right\} , \tag{6}$$

which shows that the only γ-terms that contribute are those where the γ state is either occupied or unoccupied in both $|\alpha_1 \ldots \alpha_n\rangle$ and $|\beta_1 \ldots \beta_m\rangle$ simultaneously. This means that $m = n$, and that $\{\alpha_1 \ldots \alpha_n\}$ is some permutation P of $\{\beta_1 \ldots \beta_n\}$. As a consequence, $\xi_{\alpha_1} \ldots \xi_{\alpha_n} \xi^*_{\beta_1} \ldots \xi^*_{\beta_m} = (-1)^P \xi_{\alpha_1} \ldots \xi_{\alpha_n} \xi^*_{\alpha_1} \ldots \xi^*_{\alpha_m}$. Observing that an even number of pair exchanges is required to bring the product in Eq. (5) to the form in Eq. (6), we find that each transformation contributes a factor of 1, and the final value of the expression is $(-1)^P$. It is a known result of second quantization that this is exactly the value of the overlap between the two considered many-particle states: $(-1)^P = \langle \alpha_1 \ldots \alpha_n | \beta_1 \ldots \beta_n \rangle$. This proves the key equality:

$$\langle \alpha_1 \ldots \alpha_n | A | \beta_1 \ldots \beta_n \rangle = \langle \alpha_1 \ldots \alpha_n | \beta_1 \ldots \beta_n \rangle \, ,$$

for any two vectors $|\alpha_1 \dots \alpha_n\rangle$ and $|\beta_1 \dots \beta_m\rangle$ of the basis of the Fock space. This is nothing other than a proof of the following closure relation for fermions in the coherent state representation:

$$\int \prod_\alpha d\xi_\alpha^* \, d\xi_\alpha \, e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \, |\xi\rangle\langle\xi| = 1. \tag{7}$$

This completeness relation in turn provides us with a very useful expression for the trace of operators: Considering that matrix elements between vectors of the Fock space and coherent states involve Grassmann numbers, we know that $\langle\psi_i|\xi\rangle \, \langle\xi|\psi_j\rangle = \langle-\xi|\psi_j\rangle \, \langle\psi_i|\xi\rangle$. Using this, and considering a complete set $\{|n\rangle\}$ of states in the Fock space, we may express the trace of an operator A as follows:

$$\begin{aligned}
\mathrm{Tr}\{A\} &= \sum_n \langle n|A|n\rangle \\
&= \int \prod_\alpha d\xi_\alpha^* \, d\xi_\alpha \, e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \sum_n \langle n|\xi\rangle \; \langle\xi|A|n\rangle \\
&= \int \prod_\alpha d\xi_\alpha^* \, d\xi_\alpha \, e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \, \langle-\xi|A \sum_n |n\rangle \, \langle n|\xi\rangle \\
&= \int \prod_\alpha d\xi_\alpha^* \, d\xi_\alpha \, e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \, \langle-\xi|A|\xi\rangle \, .
\end{aligned} \tag{8}$$

The completeness relation Eq. (7) also provides us with an elegant Grassmann coherent state representation of any ket $|\psi\rangle$: defining $\psi(\xi^*) \equiv \langle\xi|\psi\rangle$, we get

$$|\psi\rangle = \int \prod_\alpha d\xi_\alpha^* \, d\xi_\alpha \, e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \psi(\xi^*) \, |\xi\rangle \, . \tag{9}$$

Just as it is useful to know how the operators $\hat{x}$ and $\hat{p}$ act in coordinate representation, it is useful to have a clear idea of how the creation and annihilation operators act in the coherent state representation. We can apply relations (2) and (3) to the above expression, in order to obtain directly:

$$\begin{aligned}
\langle\xi|a_\alpha|\psi\rangle &= \frac{\partial}{\partial\xi_\alpha^*}\psi(\xi^*) \\
\langle\xi|a_\alpha^\dagger|\psi\rangle &= \xi_\alpha^* \psi(\xi^*).
\end{aligned} \tag{10}$$

In other words, the operators a_α and $a_\alpha^\dagger$ are represented by $\dfrac{\partial}{\partial\xi_\alpha^*}$ and ξ_α^* respectively.

Finally, let us note that the expression for the matrix element of a normal-ordered operator A (i.e., an operator written in such a way that all creation operators are to the left of the annihilation operators), takes a particularly simple form: using again relations (2) and (3), together with the expression for the overlap between coherent states (4), we immediately find

$$\langle\xi|A\big(a^\dagger_\alpha, a_\alpha\big)|\xi'\rangle = e^{\sum_\alpha \xi^*_\alpha \xi'_\alpha} A(\xi^*_\alpha, \xi'_\alpha). \tag{11}$$

For example, the expectation value of the number of particles in a state $|\xi\rangle$ is

$$\begin{aligned}\left\langle \hat{N} \right\rangle &= \frac{\langle\xi|\hat{N}|\xi\rangle}{\langle\xi|\xi\rangle} \\ &= \sum_\alpha \frac{\langle\xi|a^\dagger_\alpha a_\alpha|\xi\rangle}{\langle\xi|\xi\rangle} \\ &= \sum_\alpha \xi^*_\alpha \xi_\alpha,\end{aligned}$$

which is not a fixed number, but more surprisingly, is not a real number either.

We conclude this section with a short comment on the concept of fermionic coherent states. Coherent states for bosons are usually identified as those which correspond to the classical limit of quantum mechanics (e.g. in the harmonic oscillator system). Fermion coherent states do not lend themselves to this interpretation: they are not part of the fermion Fock space, are not physically observable, and do not correspond to any form of classical field. Nevertheless, as sometimes occurs in other branches of physics, they are a useful and efficient formal tool, in this case for unifying many-fermion and many-boson problems. One notable consequence of this difference in nature between bosonic and fermionic coherent states appears when one applies the stationary phase approximation. This approximation applied to a bosonic expression yields an expansion around a physical classical field configuration. There is no such thing for fermions, and this means that in order to make such an approximation useful, one has to integrate out explicitly the fermionic degrees of freedom.

III. FUNCTIONAL INTEGRAL FORMALISM

The functional integral representation of many-particle systems dates back to the seminal work of Dirac[14], extensively developed by Feynman[15–17]. Its appeal lies partially in the fact that the partition function can be expressed as an integral over field configurations. This in turn lends itself readily to useful physical approximations, and a very intuitive description of the system. We will now consider the extension of this approach to a general many-particle system described using the second quantization formalism, and use the coherent states in place of the momentum and position eigenstates, which lead to the standard derivation of the Feynman path integral expressions. The derivations follow the textbook by Negele and Orland[12].

A. Time evolution operator

An intuitive way to introduce this functional integral representation is to calculate the matrix element of the evolution operator between one initial coherent state $|\phi_i\rangle$ at time t_i, with components $\phi_{\alpha,i}$ – in terms of the expansion described in Eq. (1) –, and a final state $\langle\phi_f|$ at time t_f, with components $\phi^*_{\alpha,f}$. Formally, for a time-independent Hamiltonian H, we have:

$$\mathcal{U}\big(\phi^*_{\alpha,f}, t_f; \phi_{\alpha,i}, t_i\big) = \langle\phi_f|e^{-\frac{i}{\hbar}H(t_f-t_i)}|\phi_i\rangle \tag{12}$$

We may, with no loss of generality, assume the Hamiltonian to be normal-ordered. In that case, it can be seen that

$$\exp\Big(-i\frac{\epsilon}{\hbar}H\big(a^\dagger, a\big)\Big) =: \exp\Big(-i\frac{\epsilon}{\hbar}H\big(a^\dagger, a\big)\Big) : +\mathcal{O}\big(\epsilon^2\big),$$

where $: A :$ denotes the normal-ordered form of operator A.

We may split the time interval into M intervals of length $\epsilon = \dfrac{t_f - t_i}{M}$, of the form $[t_k, t_{k+1}]$. To this end, we introduce $t_k = t_i + k\epsilon$, for $k \in [0, \ldots, M]$. With these definitions, $t_0 = t_i$ and $t_M = t_f$. The closure relation Eq.(7), can then be used at each internal time step t_k, $k \in [1, \ldots, M-1]$:

$$\int \prod_\alpha d\phi^*_{\alpha,k}\, d\phi_{\alpha,k}\, e^{-\sum_\alpha \phi^*_{\alpha,k}\,\phi_{\alpha,k}}\, |\phi_k\rangle\langle\phi_k| = 1,$$

For notational convenience, we define $\phi_{\alpha,0} \equiv \phi_{\alpha,i}$ and $\phi_{\alpha,f} \equiv \phi_{\alpha,M}$. With these, we obtain:

$$\begin{aligned}
&\mathcal{U}\big(\phi^*_{\alpha,f}, t_f; \phi_{\alpha,i}, t_i\big) = \langle\phi_f|e^{-\frac{i}{\hbar}H(t_f-t_i)}|\phi_i\rangle \\
&= \lim_{M\to\infty} \int \prod_{k=1}^{M-1}\prod_\alpha d\phi^*_{\alpha,k}\, d\phi_{\alpha,k}\, e^{-\sum_{k=1}^{k=M-1}\sum_\alpha \phi^*_{\alpha,k}\,\phi_{\alpha,k}} \\
&\times \prod_{k=1}^{M} \langle\phi_k|: \exp\Big(-i\frac{\epsilon}{\hbar}H\big(a^\dagger, a\big)\Big) : +\mathcal{O}\big(\epsilon^2\big)|\phi_{k-1}\rangle \\
&= \lim_{M\to\infty} \int \prod_{k=1}^{M-1}\prod_\alpha d\phi^*_{\alpha,k}\, d\phi_{\alpha,k}\, e^{-\sum_{k=1}^{k=M-1}\sum_\alpha \phi^*_{\alpha,k}\,\phi_{\alpha,k}} \\
&\times \exp\left[\sum_{k=1}^{M}\left(\sum_\alpha \phi^*_{\alpha,\,k}\phi_{\alpha,\,k-1} - \frac{i\epsilon}{\hbar}H\big(\phi^*_{\alpha,\,k},\, \phi_{\alpha,\,k-1}\big)\right)\right],
\end{aligned} \tag{13}$$

where the crucial expression Eq. (11) was used to obtain the last line.

By analogy with the Feynman path integral formalism, which defines trajectories in real space, it is convenient to introduce the concept of a trajectory $\phi_\alpha(t)$ in the space of coherent states, as the limit, as $M \to \infty$, of the set $\{\phi_{\alpha,0}, \ldots, \phi_{\alpha,M}\}$. This naturally induces us to switch to a continuous notation, in which the following definitions are used:

$$\begin{aligned} \phi_{\alpha,k} &\equiv \phi_\alpha(t) \\ \frac{\phi_{\alpha,k} - \phi_{\alpha,k-1}}{\epsilon} &\equiv \frac{\partial}{\partial t}\phi_\alpha(t) \\ H\left(\phi^*_{\alpha,k},\, \phi_{\alpha,k-1}\right) &\equiv H(\phi^*_\alpha(t),\, \phi_\alpha(t)) \end{aligned}$$

With this notation, the exponent of the integrand in the last line of Eq. (13) becomes

$$\begin{aligned} &\sum_\alpha \phi^*_{\alpha,M}\phi_{\alpha,M-1} - \frac{i\epsilon}{\hbar} H\left(\phi^*_{\alpha,M},\, \phi_{\alpha,M-1}\right) \\ &+ i\epsilon \sum_{k=1}^{M-1}\left(i\sum_\alpha \phi^*_{\alpha,k}\left(\frac{\phi_{\alpha,k}-\phi_{\alpha,k-1}}{\epsilon}\right) - \frac{1}{\hbar} H\left(\phi^*_{\alpha,k},\, \phi_{\alpha,k-1}\right)\right) \\ &\underset{\epsilon\to 0}{=} \sum_\alpha \phi^*_\alpha(t_f)\phi_\alpha(t_f) + \frac{i}{\hbar}\int_{t_i}^{t_f} dt \left[\sum_\alpha i\hbar\phi^*_\alpha(t)\frac{\partial}{\partial t}\phi_\alpha(t) - H(\phi^*_\alpha(t),\, \phi_\alpha(t))\right] \\ &= \sum_\alpha \phi^*_\alpha(t_f)\phi_\alpha(t_f) + \frac{i}{\hbar}\int_{t_i}^{t_f} dt L(\phi^*_\alpha(t),\, \phi_\alpha(t)), \end{aligned} \tag{14}$$

where L stands for the Lagrangian operator: $L \equiv i\hbar\dfrac{\partial}{\partial t} - H$.

As a conclusion, we have obtained the functional integral representation of the matrix element of the evolution operator in the coherent state representation:

$$\begin{aligned} \mathcal{U}\left(\phi^*_{\alpha,f}, t_f; \phi_{\alpha,i}, t_i\right) = &\int_{\phi_\alpha(t_i)\equiv\phi_{\alpha,i}}^{\phi^*_\alpha(t_f)\equiv\phi^*_{\alpha,f}} \mathcal{D}[\phi^*_\alpha(t),\, \phi_\alpha(t)] e^{\sum_\alpha \phi^*_\alpha(t_f)\phi_\alpha(t_f)} \\ &\times \exp\left\{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\left[\sum_\alpha i\hbar\phi^*_\alpha(t)\frac{\partial}{\partial t}\phi_\alpha(t) - H(\phi^*_\alpha(t),\, \phi_\alpha(t))\right]\right\}, \end{aligned} \tag{15}$$

where

$$\int_{\phi_\alpha(t_i)\equiv\phi_{\alpha,i}}^{\phi^*_\alpha(t_f)\equiv\phi^*_{\alpha,f}} \mathcal{D}[\phi^*_\alpha(t),\, \phi_\alpha(t)] \equiv \lim_{M\to\infty}\int \prod_{k=1}^{M-1}\prod_\alpha d\phi^*_{\alpha,k},\, d\phi_{\alpha,k}.$$

A few remarks are in order at this point with regards to this final expression Eq. (15). First, in the discrete expression, $\phi_{\alpha,0}$ and $\phi^*_{\alpha,M}$ are present, as the states for which the matrix element of the evolution operator is calculated, but neither $\phi^*_{\alpha,0}$ nor $\phi_{\alpha,M}$ appear. Moreover, all variables of the type $\phi^*_{\alpha,k}$ and $\phi_{\alpha,k}$ for $k \in \{1, \ldots, M-1\}$ are integrated over. When considering the trajectory notation, note that $\phi^*_\alpha(t)$ is associated to $\phi^*_{\alpha,\,k}$, while $\phi_\alpha(t)$ is associated to $\phi^*_{\alpha,\,k-1}$. Therefore, carried over to the trajectory notation, the previous observation means that $\phi^*_\alpha(t_f)$ and $\phi_\alpha(t_i)$ are specified by the matrix element we wish to calculate, i.e., the boundary conditions of the trajectory, while $\phi^*_\alpha(t_i)$ and $\phi_\alpha(t_f)$ are internal variables over which integration is carried out.

Second, if one considers the corresponding derivation applied for a single particle in the coordinate basis, one obtains the Feynman path integral:

$$\mathcal{U}(x_f, t_f;\, x_i, t_i) = \int\limits_{(x_i,t_i)}^{(x_f,t_f)} \mathcal{D}[x(t)][p(t)] \exp\left\{ \frac{i}{\hbar} \int\limits_{t_i}^{t_f} dt \left[p(t) \frac{\partial}{\partial t} x(t) - H(p(t),\, x(t)) \right] \right\},$$

which, in spite of a strong formal similarity with Eq .(15), contains a very important difference: in the Feynman path integral expression, the factor $\frac{1}{\hbar}$ appears as a constant factor in front of the entire exponent. As a result, the stationary phase approximation corresponds to the classical limit. In the present formalism of Eq. (15), a factor $\hbar$ appears inside the expression for the Lagrangian itself, in addition to the same global $\frac{1}{\hbar}$ factor, so that the same stationary phase approximation leads to a result which differs from the classical limit.

B. Partition function for a many-body fermion system

The partition function for a many-particle system is given by[18]

$$\begin{aligned} Z = \mathrm{Tr}\, e^{-\beta\left(\hat{H}-\mu\hat{N}\right)} &= \int dx\, \langle x| e^{-\beta\left(\hat{H}-\mu\hat{N}\right)} |x\rangle \\ &= \int \prod_\alpha d\phi^*_\alpha\, d\phi_\alpha\, e^{-\sum_\alpha \phi^*_\alpha \phi_\alpha} \langle -\phi| e^{-\beta\left(\hat{H}-\mu\hat{N}\right)} |\phi\rangle\,, \end{aligned} \tag{16}$$

where the last line of Eq. (8) was used, with A replaced by the Hamiltonian in the grand canonical ensemble.

This relation may be seen as the sum of the diagonal matrix elements of the time evolution operator, after a Wick rotation to imaginary time has been applied. Under this transformation, the integration domain becomes the imaginary time interval $\tau_f - \tau_i = \beta\hbar$. With this picture in mind, it is clear that all the steps in the derivation of Eq. (15) may be repeated, using imaginary time variables, by replacing t with the variable $-i\tau$, with τ imaginary time. If this is done, then Eq. (15) becomes (replace dt by $-id\tau$, and $\frac{\partial}{\partial t}$ by $i\frac{\partial}{\partial \tau}$):

$$
\begin{aligned}
Z = & \int\limits_{\phi_\alpha(\beta)=-\phi_\alpha(0)} \mathcal{D}[\phi^*_\alpha(\tau),\, \phi_\alpha(\tau)] \\
& \exp\left\{-\int\limits_0^\beta d\tau \left[\sum_\alpha \phi^*_\alpha(\tau)\left(\frac{\partial}{\partial\tau} - \mu\right)\phi_\alpha(\tau) + H(\phi^*_\alpha(\tau),\, \phi_\alpha(\tau))\right]\right\},
\end{aligned} \tag{17}
$$

where the boundary term $e^{\sum\limits_\alpha \phi^*_\alpha(t_f)\phi_\alpha(t_f)}$ (a number) has been dropped for simplicity, with no loss of generality, and units where $\hbar = 1$ have been used (and will be used throughout the rest of this section). This expression allows us to introduce the action in this representation as

$$
\begin{aligned}
S[\phi^*_\alpha(\tau),\, \phi_\alpha(\tau)] &\equiv \int\limits_0^\beta d\tau \left[\sum_\alpha \phi^*_\alpha(\tau)\left(\frac{\partial}{\partial\tau} - \mu\right)\phi_\alpha(\tau) + H(\phi^*_\alpha(\tau),\, \phi_\alpha(\tau))\right] \\
&= \int\limits_0^\beta d\tau\, L(\phi^*_\alpha(\tau),\, \phi_\alpha(\tau)),
\end{aligned} \tag{18}
$$

where $L(\phi^*_\alpha(\tau),\, \phi_\alpha(\tau))$ is the imaginary time Lagrangian for the problem at hand.

Note that in expression (17), the integration is done over trajectories satisfying antiperiodic boundary conditions for the Grassmann variables. The problem has thus been formally reduced to a quadrature, and the last remaining step in order to apply this result consists in developing techniques which allow the evaluation of the expression (17).

IV. LAGRANGIAN EXPRESSION FOR SELECTED MODELS

A. Non-interacting system

As a preparation for the study of the Anderson and Hubbard models, it is useful to evaluate the action for a system of non-interacting particles described by a one-body Hamiltonian. In this section we follow the presentation by Negele and Orland[12].

For convenience, we choose a basis in which H_0 is diagonal. The partition function for a many-particle system is given by Eq. (16). Thus the discrete expression for the functional integral form of the partition function reads

$$
\begin{aligned}
H_0 &= \sum_\alpha \epsilon_\alpha a_\alpha^\dagger a_\alpha, \\
Z_0 &= \lim_{M\to\infty} \prod_\alpha \left[\prod_{k=1}^{n} \int d\phi_{\alpha,k}^* d\phi_{\alpha,k} e^{-\sum_{j,k=1}^{M} \phi_{\alpha,j}^* S_{jk}^{(\alpha)} \phi_{\alpha,k}} \right] \\
&= \lim_{M\to\infty} \prod_\alpha \det S^{(\alpha)},
\end{aligned} \tag{19}
$$

where

$$
S^{(\alpha)} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & a \\ -a & 1 & 0 & \ddots & 0 & 0 \\ 0 & -a & 1 & \ddots & 0 & 0 \\ 0 & 0 & -a & \ddots & 0 & 0 \\ \vdots & 0 & 0 & \ddots & 1 & 0 \\ \vdots & 0 & 0 & \ddots & -a & 1 \end{bmatrix}, \quad \phi_\alpha = \begin{bmatrix} \phi_{\alpha,1} \\ \phi_{\alpha,2} \\ \vdots \\ \phi_{\alpha,M}, \end{bmatrix} \tag{20}
$$

$$
a = 1 - \frac{\beta}{M}(\epsilon_\alpha - \mu),
$$

with the convention that the time index increases with increasing row and column index.

The determinant of $S^{(\alpha)}$ may be evaluated by expanding by minors along the first row:

$$
\begin{aligned}
\lim_{M\to\infty} \det S^{(\alpha)} &= \lim_{M\to\infty} \left[1 + (-1)^{M-1} a(-a)^{M-1}\right] = \lim_{M\to\infty} \left[1 + a^M\right] \\
&= \lim_{M\to\infty} \left[1 + \left(1 - \frac{\beta(\epsilon_\alpha - \mu)}{M}\right)^M\right] \\
&= 1 + e^{-\beta(\epsilon_\alpha - \mu)}.
\end{aligned} \tag{21}
$$

Substitution into Eq. (19) yields the familiar expression for the partition function of a system of non-interacting particles:

$$
Z_0 = \prod_\alpha \left(1 + e^{-\beta(\epsilon_\alpha - \mu)}\right).
$$

Equipped with these results, we may turn to the evaluation of the single-particle Green's function for non-interacting particles, $\mathcal{G}_0$. Let τ_q correspond to the time $q\dfrac{\beta}{M}$, and τ_r correspond to the time $r\dfrac{\beta}{M}$, for integers q and r. We recall the general result about gauss integrals:

$$
\frac{1}{(2\pi)^{\frac{n}{2}}} \int dx_1 \ldots dx_n e^{-\frac{1}{2} x_i A_{ij} x_j + x_i J_i} = [\det A]^{-\frac{1}{2}} e^{\frac{1}{2} J_i A_{ij}^{-1} J_j}, \tag{22}
$$

where A is a real symmetric definite positive matrix, and summation over repeated indices is assumed. A similar identity holds for a Gaussian integral over complex variables, in the form:

$$\int \prod_{i=1}^{n} \frac{dx_i^* dx_i}{2i\pi} e^{-x_i^* H_{ij} x_j + J_i^* x_i + J_i x_i^*} = [\det H]^{-1} e^{J_i^* H_{ij}^{-1} J_j}, \tag{23}$$

where H is a Hermitian matrix.

Thus, we obtain

$$\begin{aligned}
\mathcal{G}_0(\alpha\tau_q|\gamma\tau_r) &= -\left\langle T_\tau a_\alpha(\tau_q) a_\gamma^\dagger(\tau_r)\right\rangle \\
&= -\frac{1}{Z_0} \operatorname{Tr}\left[e^{-\beta(H-\mu N)} T_\tau a_\alpha(\tau_q) a_\gamma^\dagger(\tau_r)\right] \\
&= -\frac{1}{Z_0} \lim_{M\to\infty} \int \prod_\delta \prod_{k=1}^{M} d\phi_{\delta,k}^* d\phi_{\delta,k} e^{-\sum\limits_{j,k=1}^{M} \phi_{\delta,j}^* S_{jk}^{(\delta)} \phi_{\delta,k}} \phi_{\alpha,q}\phi_{\gamma,r}^* \\
&= -\delta_{\alpha\gamma} \frac{\int \prod\limits_k d\phi_k^* d\phi_k e^{-\sum\limits_{j,k=1}^{M} \phi_j^* S_{jk}^{(\alpha)} \phi_k} \phi_q \phi_r^*}{\int \prod\limits_k d\phi_k^* d\phi_k e^{-\sum\limits_{j,k=1}^{M} \phi_j^* S_{jk}^{(\alpha)} \phi_k}} \\
&= -\delta_{\alpha\gamma} \frac{\partial^2}{\partial J_q^* \partial J_r} \left.\frac{\int \prod\limits_k d\phi_k^* d\phi_k e^{-\sum\limits_{j,k=1}^{M} \phi_j^* S_{jk}^{(\alpha)} \phi_k + \sum i(J_i^*\phi_i + \phi^* J_i)}}{\int \prod\limits_k d\phi_k^* d\phi_k e^{-\sum\limits_{j,k=1}^{M} \phi_j^* S_{jk}^{(\alpha)} \phi_k}}\right|_{J=J^*=0} \\
&= -\delta_{\alpha\gamma} \frac{\partial^2}{\partial J_q^* \partial J_r} \left. e^{\sum\limits_{j,k=1}^{M} J_j^* S_{jk}^{(\alpha)^{-1}} J_k}\right|_{J=J^*=0} \\
&= -\delta_{\alpha\gamma} S_{qr}^{(\alpha)^{-1}},
\end{aligned} \tag{24}$$

where repeated use was made of Eq. (22).

The matrix S is defined in Eq. (20). It is straightforward to check that its inverse is given by the following expression:

$$S^{(\alpha)^{-1}} = \frac{1}{1+a^M}\begin{bmatrix} 1 & -a^{M-1} & -a^{M-2} & \cdots & -a \\ a & 1 & -a^{M-1} & \cdots & -a^2 \\ a^2 & a & 1 & \cdots & -a^3 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ a^{M-3} & \ddots & \ddots & \ddots & -a^{M-2} \\ a^{M-2} & a^{M-3} & \ddots & \ddots & -a^{M-1} \\ a^{M-1} & a^{M-2} & a^{M-3} & \cdots & 1 \end{bmatrix}. \tag{25}$$

For $q \geq r$, we have

$$\begin{aligned} \lim_{M\to\infty} S_{qr}^{(\alpha)^{-1}} &= \lim_{M\to\infty} \frac{a^{q-r}}{1+a^M} \\ &= \lim_{M\to\infty} \left(1 - \frac{\beta}{M}(\epsilon_\alpha - \mu)\right)^{q-r} \left(1 - \frac{1}{\left(1 - \frac{\beta}{M}(\epsilon_\alpha - \mu)\right)^{-M} + 1}\right) \\ &= e^{-(\epsilon_\alpha-\mu)(\tau_q-\tau_r)} \left(1 - \frac{1}{e^{\beta(\epsilon_\alpha-\mu)}+1}\right) \\ &= e^{-(\epsilon_\alpha-\mu)(\tau_q-\tau_r)}(1-n_\alpha), \end{aligned} \tag{26}$$

where n_α it the Fermi-Dirac distribution:

$$n_\alpha = \frac{1}{1+e^{\beta(\epsilon_\alpha-\mu)}}.$$

The result for $q \leq r$ is obtained similarly:

$$\begin{aligned} \lim_{M\to\infty} S_{qr}^{(\alpha)^{-1}} &= \lim_{M\to\infty} -\frac{a^{M+q-r}}{1+a^M} \\ &= \lim_{M\to\infty} \left(1 - \frac{\beta}{M}(\epsilon_\alpha - \mu)\right)^{q-r} \left(\frac{-1}{\left(1 - \frac{\beta}{M}(\epsilon_\alpha - \mu)\right)^{-M} + 1}\right) \\ &= -e^{-(\epsilon_\alpha-\mu)(\tau_q-\tau_r)} n_\alpha. \end{aligned} \tag{27}$$

With these results, the case in which creation and annihilation operators act at equal times need to be considered. Using the fact that the time-ordered product is defined to be equal to a normal ordered product at equal time, we find that the time-ordered product may be written $T_\tau\left[a_\beta(\tau)a_\alpha^\dagger(\tau)\right] = -a_\alpha^\dagger(\tau)a_\beta(\tau) = a_\beta(\tau)a_\alpha^\dagger(\tau) - \delta_{\alpha\beta}$, in which case the evolution operator gives rise to the term

$$
\begin{aligned}
&|\phi_{k+1}\rangle\langle\phi_{k+1}|\, e^{-\epsilon H} a_\alpha\, |\phi_k\rangle\langle\phi_k|\, a_\beta^\dagger e^{-\epsilon H}\, |\phi_{k-1}\rangle\langle\phi_{k-1}| \ldots \\
&\qquad\qquad = |\phi_{k+1}\rangle\, e^{-\epsilon H\left(\phi_{k+1}^*,\phi_k\right)} \phi_{\alpha,k}\phi_{\beta,k}^* e^{-\epsilon H\left(\phi_k^*,\phi_{k-1}\right)}\, \langle\phi_{k-1}| \ldots,
\end{aligned}
$$

where ϕ_α and ϕ_β are evaluated at equal times. Thus, following the derivation of Eq. (24), $\left\langle T_\tau a_\alpha(\tau)a_\alpha^\dagger(\tau)\right\rangle = S_{r,r}^{-1} - 1 = -n_\alpha$.

Combining the obtained results, the single-particle Green's function can be written as

$$
\begin{aligned}
\mathcal{G}_0(\alpha\tau|\alpha'\tau') &= -\left\langle T_\tau a_\alpha(\tau)a_{\alpha'}^\dagger(\tau')\right\rangle \\
&= -\delta_{\alpha\alpha'} e^{-(\epsilon_\alpha-\mu)(\tau-\tau')}\{\theta(\tau-\tau'-\eta)(1-n_\alpha) - \theta(\tau-\tau'+\eta)n_\alpha\},
\end{aligned}
\tag{28}
$$

where η is a positive infinitesimal which allows the correct treatment of the case $\tau = \tau'$. With this expression, it is easily verified that

$$
-\sum_{\alpha_2}[\delta_{\alpha_1\alpha_2}(\partial_{\tau_2}-\mu) + \langle\alpha_1|H_0|\alpha_2\rangle]\mathcal{G}_0(\alpha_2\tau_2|\alpha_3\tau_3) = \delta_{\alpha_1\alpha_2}\delta(\tau_2-\tau_3).
$$

Thus, for a non-interacting system, we get

$$
\mathcal{G}_0^{-1}(\alpha_1\tau_1|\alpha_2\tau_2) = -[\delta_{\alpha_1\alpha_2}(\partial_{\tau_1}-\mu) + \langle\alpha_1|H_0|\alpha_2\rangle]\delta(\tau_1-\tau_2).
$$

Identifying the relevant terms of the expression above with those of Eq. (18), and using the fact that the diagonal basis of the non-interacting Hamiltonian has been used, we find that the action for the non-interaction system may be written as

$$
\begin{aligned}
S[\phi_\alpha^*(\tau),\, \phi_\alpha(\tau)] &= \int_0^\beta d\tau\, L(\phi_\alpha^*(\tau),\, \phi_\alpha(\tau)) \\
&\equiv -\int_0^\beta d\tau \int_0^\beta d\tau' \left[\sum_\alpha \phi_\alpha^*(\tau)\mathcal{G}_0^{-1}(\alpha;\tau-\tau')\phi_\alpha(\tau')\right],
\end{aligned}
\tag{29}
$$

where $L(\phi_\alpha^*(\tau),\, \phi_\alpha(\tau))$ is the imaginary time Lagrangian for the model.

B. Single impurity Anderson model

The Hamiltonian of the single impurity Anderson model can be written as:

$$\begin{aligned}
H &= H_\mu + H_U + H_{\text{bath}} + H_{\text{mix}}, \\
H_\mu &= -\mu \sum_\sigma \hat{n}_\sigma, \\
H_U &= U \hat{n}_\uparrow \hat{n}_\downarrow, \\
H_{\text{mix}} &= \sum_{\boldsymbol{k}\sigma} V_{\boldsymbol{k}\sigma} c_\sigma^\dagger a_{\boldsymbol{k}\sigma} + \text{H.c.}, \\
H_{\text{bath}} &= \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} a_{\boldsymbol{k}\sigma}^\dagger a_{\boldsymbol{k}\sigma},
\end{aligned} \tag{30}$$

where the operators $\hat{n}_\sigma$ and $c_\sigma^{(\dagger)}$ act on the impurity site, whose Hilbert space is spanned by the four states $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$. We introduce the local part of the Hamiltonian

$$H_{\text{loc}} = H_\mu + H_U,$$

which describes the on site interaction, and the influence of the chemical potential, on the impurity site. The impurity is coupled to a bath described by H_{bath}, via the terms present in H_{mix}.

As presented in Sec. III A, we may represent the system with the help of a path integral which involves the action along all the possible paths. In the case of the Hamiltonian of Eq. (30), the expression derived in Eq. (18) takes the form

$$\begin{aligned}
S &= \int_0^\beta d\tau \sum_\alpha \left(\phi_\alpha^* \partial_\tau \phi_\alpha + H(\phi_\alpha^*, \phi_\alpha)\right) \\
&= \int_0^\beta d\tau \sum_\alpha \left[\phi_\alpha^* (\partial_\tau - \mu)\phi_\alpha + H_U(\phi_\alpha^*, \phi_\alpha) + H_{\text{mix}}(\phi_\alpha^*, \phi_\alpha) + H_{\text{bath}}(\phi_\alpha^*, \phi_\alpha)\right].
\end{aligned}$$

In this expression, the bath operators, even though they are coupled to the impurity site operators, appear only in quadratic terms, and may thus be integrated out, leaving us with the impurity site operators, on which we wish to focus. The terms coming from $H_{\text{mix}}(\phi^*, \phi)$ and $H_{\text{bath}}(\phi^*, \phi)$ can be handled if we use the expression for a Gaussian integral over Grassmann variables, given in Eq. (22), with $A_{ij} \equiv \delta_{ij}(\partial_\tau - \epsilon_j)$, and $J \equiv V_l \phi_0$, and $(\phi_{0\uparrow}^*, \phi_{0\uparrow}, \phi_{0\downarrow}^*, \phi_{0\downarrow})$ the four Grassmann generators associated with the impurity site. The term $\det A$ coming from the expression for the Gaussian integral reduces to an additive term $S_{\rm bath}$ in the action, which we can drop in the partition function expression, since it is tantamount to a shift in the free energy. With this, we obtain:

$$
\begin{aligned}
S &= S_{\rm eff} + S_{\rm bath}, \\
Z &= \int \prod_{\sigma} \mathcal{D}\phi^*_{0\sigma} \mathcal{D}\phi_{0\sigma} e^{-S_{\rm eff}}, \\
S_{\rm eff} &= \int_0^\beta d\tau \left(\sum_\sigma \phi^*_{0\sigma} \left[(\partial_\tau - \mu) + \sum_{lm} V^*_l \left[(\partial_\tau - \epsilon_l)^{-1} \right]_{lm} V_m \right] \phi_{0\sigma} + H_U(\phi^*_{0\uparrow}, \phi^*_{0\downarrow}, \phi_{0\uparrow}, \phi_{0\downarrow}) \right) \\
&= \int_0^\beta d\tau \left(\sum_\sigma \phi^*_{0\sigma} \left[(\partial_\tau - \mu) + \sum_{l} V^*_l \left[(\partial_\tau - \epsilon_l)^{-1} \right]_{ll} V_l \right] \phi_{0\sigma} + H_U(\phi^*_{0\uparrow}, \phi^*_{0\downarrow}, \phi_{0\uparrow}, \phi_{0\downarrow}) \right),
\end{aligned}
$$

where the diagonal nature of the bath Hamiltonian was used to obtain the last line.

The non interacting part of this action has the form obtained in Eq. (29), with the following form of the inverse bare propagator:

$$
\begin{aligned}
\mathcal{G}_0^{-1}(i\omega_n)^{\rm AM} &= i\omega_n + \mu - \int_{-\infty}^{+\infty} d\omega \frac{\Delta(\omega)}{i\omega_n - \omega}, \\
\text{where } \Delta(\omega) &\equiv \sum_{l\sigma} |V_l|^2 \delta(\omega - \epsilon_l).
\end{aligned}
\tag{31}
$$

Considering that any problem may be studied in its Lagrangian or Hamiltonian representation, the above expression is helpful, insofar as it establishes the correspondence between the parameters of the Hamiltonian representation of the single impurity Anderson model (the sets of ϵ_l and V_l), and the parameters of its Lagrangian representation (the form of the bare propagator $\mathcal{G}_0^{-1}(i\omega_n)$ determining $S_{\rm eff}$).

C. Hubbard model

The Hamiltonian of the Hubbard model reads

$$
\begin{aligned}
H &= H_0 + \Delta H + H^{(o)}, \\
H_0 &= U\hat{n}_{0\uparrow}\hat{n}_{0\downarrow} - \mu \sum_\sigma c^\dagger_{0\sigma} c_{0\sigma}, \\
\Delta H &= -\sum_{\langle i \rangle, \sigma} t_{i0} \left(c^\dagger_{0\sigma} c_{i\sigma} + c^\dagger_{i\sigma} c_{0\sigma} \right), \\
H^{(o)} &= -\sum_{\langle i \neq 0, j \neq 0 \rangle, \sigma} t_{ij} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{H. c.} \right) + U \sum_{i \neq 0} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu \sum_{i \neq 0 \sigma} c^\dagger_{i\sigma} c_{i\sigma},
\end{aligned}
\tag{32}
$$

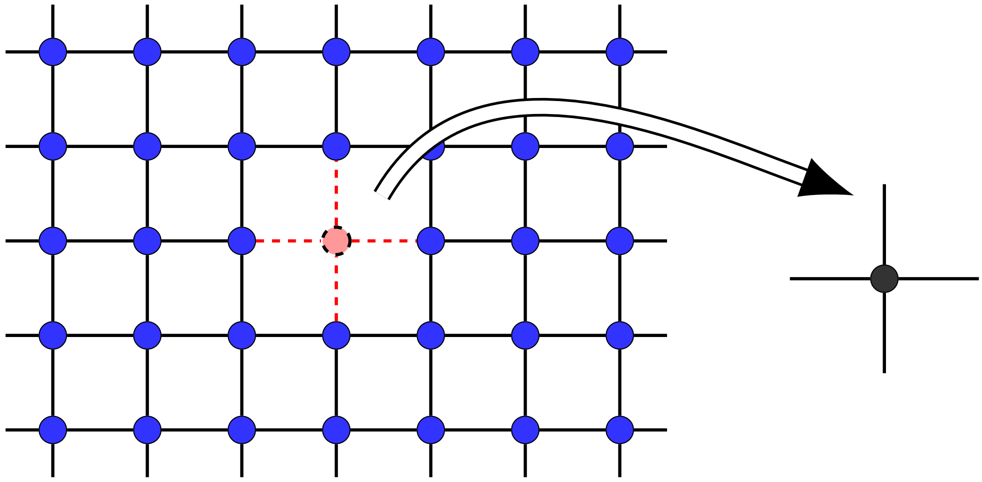

FIG. 1: In this schematic representation, the original lattice point of view is shown on the left. One site (in red) is singled out, then removed, creating a cavity in the lattice. The single site is then considered as an impurity, while the remainder of the sites are viewed as a bath, whose electrons hop into, or out from, the impurity.

where the hopping terms entering ΔH are those connecting the site 0 with its nearest neighbors, and we assume a grand-canonical ensemble with the chemical potential μ. This splitting of the Hamiltonian corresponds to the situation depicted in Fig. 1, in which one site, with index 0, is singled out. We consider the terms of the Hamiltonian which contain only operators acting on the site 0 (H_0), those which contain only operators acting on sites different from the site 0 ($H^{(o)}$, the cavity Hamiltonian), and those which connect the site 0 with other sites (ΔH).

As discussed in Sec. III A and above, we may represent the system with the help of a path integral. Using the Hamiltonian of Eq. (32), and the splitting it introduces, the expression derived in Eq. (18) takes the form

$$
\begin{aligned}
S &= S_0 + \Delta S + S^{(o)} = \int_0^\beta d\tau \sum_\alpha \left(\phi^*_\alpha \partial_\tau \phi_\alpha + H(\phi^*_\alpha, \phi_\alpha)\right), \\
S_0 &= \int_0^\beta d\tau \left[\sum_\sigma \phi^*_{0\sigma}(\partial_\tau - \mu)\phi_{0\sigma} + H_U(\phi^*_{0\uparrow}, \phi^*_{0\downarrow}, \phi_{0\uparrow}, \phi_{0\downarrow}) \right], \\
\Delta S &= -\int_0^\beta d\tau \left[\sum_{i\sigma} t_{i0}(\phi^*_{i\sigma}\phi_{0\sigma} + \phi^*_{0\sigma}\phi_{i\sigma}) \right], \\
S^{(o)} &= \int_0^\beta d\tau \Bigg[\sum_{i\neq 0,\, \sigma} \phi^*_{i\sigma}(\partial_\tau - \mu)\phi_{i\sigma} \\
&\quad - \sum_{i\neq 0,\, j\neq 0,\, \sigma} t_{ij}\left(\phi^*_{i\sigma}\phi_{j\sigma} + \phi^*_{j\sigma}\phi_{i\sigma}\right) + \sum_{i\neq 0} H_U(\phi^*_{i\uparrow}, \phi^*_{i\downarrow}, \phi_{i\uparrow}, \phi_{i\downarrow}) \Bigg],
\end{aligned}
\tag{33}
$$

From this expression, we wish to build an effective action, by explicitly integrating all degrees of freedom other than those of the site 0:

$$
\frac{1}{Z_{\text{eff}}} e^{-S_{\text{eff}}\left[\phi^*_{0\uparrow}, \phi^*_{0\downarrow}, \phi_{0\uparrow}, \phi_{0\downarrow}\right]} \equiv \frac{1}{Z} \int \prod_{i\neq 0, \sigma} \mathcal{D}\phi^*_{i\sigma} \mathcal{D}\phi_{i\sigma} e^{-S[\phi^*_{i\sigma}, \phi_{i\sigma}]}. \tag{34}
$$

In order to achieve this, we use an approach inspired by the seminal work of Metzner[2]. In that work, Metzner considers the Hubbard Hamiltonian starting from the atomic limit, and treats the kinetic energy terms as the perturbation. We use a similar functional expansion, applied to the part of the exponent that mixes the site 0 with the other sites, which proceeds as follows:

$$
\begin{aligned}
&\int \prod_{i\neq 0, \sigma} \mathcal{D}\phi^*_{i\sigma} \mathcal{D}\phi_{i\sigma} e^{-S[\phi^*_{i\sigma}, \phi_{i\sigma}]} \\
&= \int\limits_{\phi_{i\sigma}(\beta) = -\phi_{i\sigma}(0)} \mathcal{D}[\phi^*_{i\sigma},\, \phi_{i\sigma}]_{i\neq 0} \exp\left\{ -\int_0^\beta d\tau \left[\sum_{i\neq 0, \sigma} \phi^*_{i\sigma} \left(\frac{\partial}{\partial \tau}\right) \phi_{i\sigma} + H^{(o)}[\phi^*_{i\sigma},\, \phi_{i\sigma}] \right] \right\} \\
&\times \exp\left\{ -\int_0^\beta d\tau \left[\sum_{i\sigma} t_{i0}(\phi^*_{i\sigma}\phi_{0\sigma} + \phi^*_{0\sigma}\phi_{i\sigma}) \right] \right\} \\
&\times \exp\left\{ -S_0\left[\phi^*_{0\uparrow}, \phi^*_{0\downarrow}, \phi_{0\uparrow}, \phi_{0\downarrow}\right] \right\},
\end{aligned}
\tag{35}
$$

in which the part of the integral to be explicitly integrated reads

$$\begin{aligned} I = & \int\limits_{\phi_{i\sigma}(\beta)=-\phi_{i\sigma}(0)} \mathcal{D}[\phi^*_{i\sigma},\, \phi_{i\sigma}]_{i\neq 0} \exp\left\{ -\int\limits_0^\beta d\tau \left[\sum_{i\neq 0\sigma} \phi^*_{i\sigma}\left(\frac{\partial}{\partial\tau}\right)\phi_{i\sigma} + H^{(o)}[\phi^*_{i\sigma},\, \phi_{i\sigma}] \right] \right\} \\ & \times \exp\left\{ -\int\limits_0^\beta d\tau \left[\sum_{i\sigma} t_{i0}(\phi^*_{i\sigma}\phi_{0\sigma} + \phi^*_{0\sigma}\phi_{i\sigma}) \right] \right\}. \end{aligned} \tag{36}$$

In this expression, we recognize the very definition of the thermal average of the quantity in the last line[12], for the system described by the cavity Hamiltonian $H^{(o)}$:

$$I = \left\langle e^{-\int\limits_0^\beta d\tau \sum\limits_{i\sigma} t_{i0}\left(\phi^*_{i\sigma}\phi_{0\sigma} + \phi^*_{0\sigma}\phi_{i\sigma}\right)} \right\rangle_{(o)} \tag{37}$$

At this point, the aforementioned functional expansion may be carried out, applied to the exponential in the bracket[2]. We introduce $\eta_{i\sigma} \equiv t_{i0}\phi_{0\sigma}$ and obtain

$$I = \sum_{n=1}^{\infty} I_n, \tag{38}$$

with the n^{th} order term of this expansion given by

$$I_n \equiv \frac{(-1)^n}{n!} \sum_{\substack{i_1\dots i_n,\\ j_1\dots j_n,\\ \sigma_1\dots\sigma_n}} \int\limits_0^\beta \left(\prod_{i=1}^n d\tau_i\right) \eta^*_{i_1\sigma_1}\dots\eta^*_{i_n\sigma_n}\eta_{j_1\sigma_1}\dots\eta_{j_n\sigma_n} \left\langle \phi^*_{i_1\sigma_1}\dots\phi^*_{i_n\sigma_n}\phi_{j_1\sigma_1}\dots\phi_{j_n\sigma_n} \right\rangle_{(o)}. \tag{39}$$

We have used the fact that an integral over Grassmann variables is non zero only if each of the variables, over which the integration is carried out, is present in the integrand. By definition, the ensemble average $\left\langle \phi^*_{i_1\sigma_1}\dots\phi^*_{i_n\sigma_n}\phi_{j_1\sigma_1}\dots\phi_{j_n\sigma_n} \right\rangle_{(o)}$ is the n-particle Green's function of the cavity system:

$$\begin{aligned} &\mathcal{G}^{(o)}(j_1\tau_1\sigma_1,\, j_2\tau_2\sigma_2,\, \dots,\, j_n\tau_n\sigma_n | i_1\tau'_1\sigma_1,\, i_2\tau'_2\sigma_2,\, \dots,\, i_n\tau'_n\sigma_n) \equiv \\ &\qquad \left\langle \phi^*_{i_1\sigma_1}(\tau'_1)\dots\phi^*_{i_n\sigma_n}(\tau'_n)\phi_{j_1\sigma_1}(\tau_1)\dots\phi_{j_n\sigma_n}(\tau_n) \right\rangle_{(o)}, \end{aligned} \tag{40}$$

evaluated for $\tau'_i = \tau_i$, $\sigma_i = \sigma'_i$. At this point, we can introduce the decomposition of the Green's function in terms of cumulants (connected Green's functions) $C^{(o)}_m$. Each term of the sums involved in such a decomposition corresponds to a partition of $(1, \dots, n, 1', \dots, n')$ in subsets containing equal numbers of primed and unprimed variables[12], e.g.:

$$\begin{aligned} G^{(o)}_1(1|1') &= C^{(o)}_1(1|1'), \\ G^{(o)}_2(1,2|1',2') &= C^{(o)}_2(1,2|1',2') + C^{(o)}_1(1|1')C^{(o)}_1(2|2') - C^{(o)}_1(1|2')C^{(o)}_1(2|1'). \end{aligned} \tag{41}$$

In these expressions, the sign attached to each product is determined by the parity of the permutation of the primed variables with respect to the unprimed variables.

At this point, the limit of infinite dimension leads to a crucial simplification: it can be shown[1] that in this limit, the hopping needs to be properly scaled, lest the kinetic energy diverges. More precisely, the hopping parameter needs to be adjusted as $t_{ij} \propto \left(1/\sqrt{d}\right)^{|i-j|}$, where $|i-j|$ is the Manhattan distance between i and j for the cubic lattice). The insight of Georges and coworkers is that this scaling, applied to the connected Green's functions appearing in Eq. (39), considerably simplifies the expression[11]: for $n=1$, $C_1^{(o)}(1|1') \propto \left(1/\sqrt{d}\right)^{|i-j|}$, $\eta_{i\sigma} \propto \left(1/\sqrt{d}\right)^{|i|}$, while the number of terms in the sum has a $\left(d^{|i-j|}\right)^2$ dependence (there are $\simeq d^s$ sites at a given Manhattan distance s from a fixed site for large d). This means that the $n=1$ term from Eq. (39) is of order 1. A detailed study of the combined scaling of the terms for $n>1$ shows that they decay as $1/d$ or faster. Therefore, Eq. (39) simplifies to

$$I = \sum_{ij\sigma} \int_0^\beta d\tau \; \eta_{i\sigma}^* \eta_{j\sigma} \left\langle \phi_{i\sigma}^* \phi_{j\sigma} \right\rangle_{(o)} = \sum_{ij\sigma} \int_0^\beta \int_0^\beta d\tau \; d\tau' \; t_{i0} t_{j0} \phi_{0\sigma}^* G_{ij,\sigma}^{(o)}(\tau') \delta(\tau-\tau') \phi_{0\sigma}. \tag{42}$$

Noting that for $i, j \neq 0$,

$$\int\limits_{\substack{\phi_{0\sigma}(\beta) \\ =-\phi_{0\sigma}(0)}} \mathcal{D}[\phi_{0\sigma}^*, \, \phi_{0\sigma}] \eta_{i\sigma}^* \eta_{j\sigma} \left\langle \phi_{i\sigma}^* \phi_{j\sigma} \right\rangle_{(o)} = \int\limits_{\substack{\phi_{0\sigma}(\beta) \\ =-\phi_{0\sigma}(0)}} \mathcal{D}[\phi_{0\sigma}^*, \, \phi_{0\sigma}] \exp\left\{ \eta_{i\sigma}^* \eta_{j\sigma} \left\langle \phi_{i\sigma}^* \phi_{j\sigma} \right\rangle_{(o)} \right\}, \tag{43}$$

we obtain from Eq. (34) and Eq. (35)

$$\begin{aligned} S_{\text{eff}} &= \sum_{ij\sigma} \int_0^\beta \int_0^\beta d\tau \; d\tau' \; t_{i0} t_{j0} \phi_{0\sigma}^* G_{ij,\sigma}^{(o)}(\tau') \delta(\tau-\tau') \phi_{0\sigma} + S_0\left[\phi_{0\uparrow}^*, \phi_{0\downarrow}^*, \phi_{0\uparrow}, \phi_{0\downarrow}\right] \\ &= \sum_\sigma \int_0^\beta d\tau \; \Bigg\{ \Bigg(\int_0^\beta d\tau' \; \phi_{0\sigma}^* \Bigg[\partial_\tau - \mu + \sum_{ij} t_{i0} t_{j0} G_{ij,\sigma}^{(o)}(\tau') \delta(\tau-\tau') \Bigg] \phi_{0\sigma} \Bigg) \\ &\qquad\qquad + H_U(\phi_{0\uparrow}^*, \phi_{0\downarrow}^*, \phi_{0\uparrow}, \phi_{0\downarrow}) \Bigg\} \\ &\equiv \sum_\sigma \int_0^\beta d\tau \; \Bigg\{ \Bigg(- \int_0^\beta d\tau' \; \phi_{0\sigma}^* \left[\mathcal{G}_0^{-1}(\tau')^{\text{IDHM}} \delta(\tau-\tau') \right] \phi_{0\sigma} \Bigg) + H_U(\phi_{0\uparrow}^*, \phi_{0\downarrow}^*, \phi_{0\uparrow}, \phi_{0\downarrow}) \Bigg\}. \end{aligned} \tag{44}$$

The non interacting part of this action has the form obtained in Eq. (29), where the following form for the inverse bare propagator (IDHM stands for "infinite dimensional Hubbard model") is used:

$$\mathcal{G}_0^{-1}(i\omega_n)^{\text{IDHM}} = i\omega_n + \mu - \sum_{ij} t_{i0} t_{j0} G^{(o)}_{ij,\sigma}(i\omega_n). \tag{45}$$

This expression is helpful, but involves $G^{(o)}_{ij,\sigma}(i\omega_n)$, which is still not known. For a general lattice, it is possible to use an expansion of the Green's function for the full Hamiltonian in powers of the hopping matrix elements[11]. This allows to establish a relation that first appeared (without formal justification) in a work by Hubbard[19]:

$$G^{(o)}_{ij,\sigma}(i\omega_n) = G_{ij,\sigma}(i\omega_n) - \frac{G_{i0\sigma}(i\omega_n) G_{0j\sigma}(i\omega_n)}{G_{00\sigma}(i\omega_n)}, \tag{46}$$

where $G_{ij,\sigma}(i\omega_n)$ denotes the Green's function for the Hubbard model including the complete lattice.

We may introduce the quantity

$$\tilde{D}(\xi) \equiv \int_{-\infty}^{+\infty} d\epsilon \; D(\epsilon) \frac{1}{\xi - \epsilon}, \tag{47}$$

as well as the self-energy $\Sigma(i\omega_n)$, assumed to be k-independent (an assumption which has to be proven valid on its own by power counting in $1/d$[11]), and show that Eq. (46) leads to

$$\mathcal{G}_0^{-1}(i\omega_n)^{\text{IDHM}} = \Sigma(i\omega_n) + \frac{1}{\tilde{D}(i\omega_n + \mu - \Sigma(i\omega_n))}. \tag{48}$$

We may now employ Dyson's equation[18] applied to the lattice and apply the DMFT approximation, which consists in the identification of the self-energy of the lattice with that of the impurity:

$$\Sigma(i\omega_n) \underbrace{=}_{\substack{\text{DMFT}\\ \text{approximation}}} \Sigma_{\text{lattice}}(i\omega_n) \equiv \mathcal{G}_0^{-1}(i\omega_n)^{\text{IDHM}} - G^{-1\,\text{IDHM}}(i\omega_n) \tag{49}$$

to obtain

$$\begin{aligned} G^{\text{IDHM}}(i\omega_n) = \tilde{D}(i\omega_n + \mu - \Sigma(i\omega_n)) = \int_{-\infty}^{+\infty} d\epsilon \; \frac{D(\epsilon)}{i\omega_n + \mu - \epsilon - \Sigma(i\omega_n)} \\ = \sum_{\mathbf{k}\in\text{BZ}} \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma(i\omega_n)} \end{aligned} \tag{50}$$

This crucial result expresses the fact that one can identify the impurity Green's function with the momentum-averaged lattice Green's function. The latter quantity depends only on the known lattice dispersion, and on the (momentum-independent) self-energy of the impurity. This is the self-consistency condition, which can be used to solve the problem iteratively.

This result holds for a lattice in the limit of infinite coordination, a crucial ingredient used in three occasions during the derivation. First, it lead to the simplification of the expression for the action, which is limited to the $n = 1$ contribution in Eq.(39). Second, it was used to relate the Green's function for the cavity Hamiltonian and that for the full Hamiltonian in Eq. (46). Third, it is a necessary ingredient in order to prove that the self-energy is k-independent.

A comparison of the $d \to \infty$ limit versus $d = 1$ and $d = 3$ was done by Metzner and Vollhardt[1]. They compared the second order contribution to the correlation energy in the Hubbard model, defined as

$$E_2 = \frac{LU^2}{(2\pi)^{3d}} \int d\boldsymbol{k} d\boldsymbol{k'} d\boldsymbol{q} \frac{n^0_{\boldsymbol{k}\uparrow} n^0_{\boldsymbol{k'}\downarrow} \left(1 - n^0_{\boldsymbol{k}+\boldsymbol{q}\uparrow}\right)\left(1 - n^0_{\boldsymbol{k'}-\boldsymbol{q}\downarrow}\right)}{\epsilon_{\boldsymbol{k}} + \epsilon_{\boldsymbol{k'}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k'}+\boldsymbol{q}}}, \tag{51}$$

where the integrations extend over the Brillouin zone, $n^0_{\boldsymbol{k}\sigma \equiv 1}$ for $|\boldsymbol{k}| < k_{F\sigma}$ and 0 elsewhere, and L is the number of lattice sites. The result is shown in Fig. 2, and shows that the $d = \infty$ limit is a reasonable approximation to the $d = 3$ situation in this case. While in no way conclusive of the general validity or quality of the $d \to \infty$ limit, it shows that it may be an approach worth exploring, at least in the situation where $d = 3$.

V. SELF-CONSISTENCY LOOP

At this point we are in a position to devise a self-consistent scheme for solving the many-body problem represented by the Hubbard model in the limit of infinite dimensions. At step p, we assume that a trial self-energy $\Sigma_p(i\omega_n)$ is known for the isolated site (the process can be initialized for the initial step $p = 0$ with $\Sigma_p(i\omega_n) \equiv 0$, for lack of a better candidate). Given this trial function, we use Eq. (50), and obtain the lattice Green's function at iteration p (note the change of notation, from G^{IDHM} to G_{lat}, following the DMFT convention which highlights the back and forth movement between the "lattice" and the "impurity" points of view, illustrated in Fig. 3):<

$$G_{lat,p}(i\omega_n) = \sum_{\mathbf{k}\in \mathrm{BZ}} \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_p(i\omega_n)}, \tag{52}$$

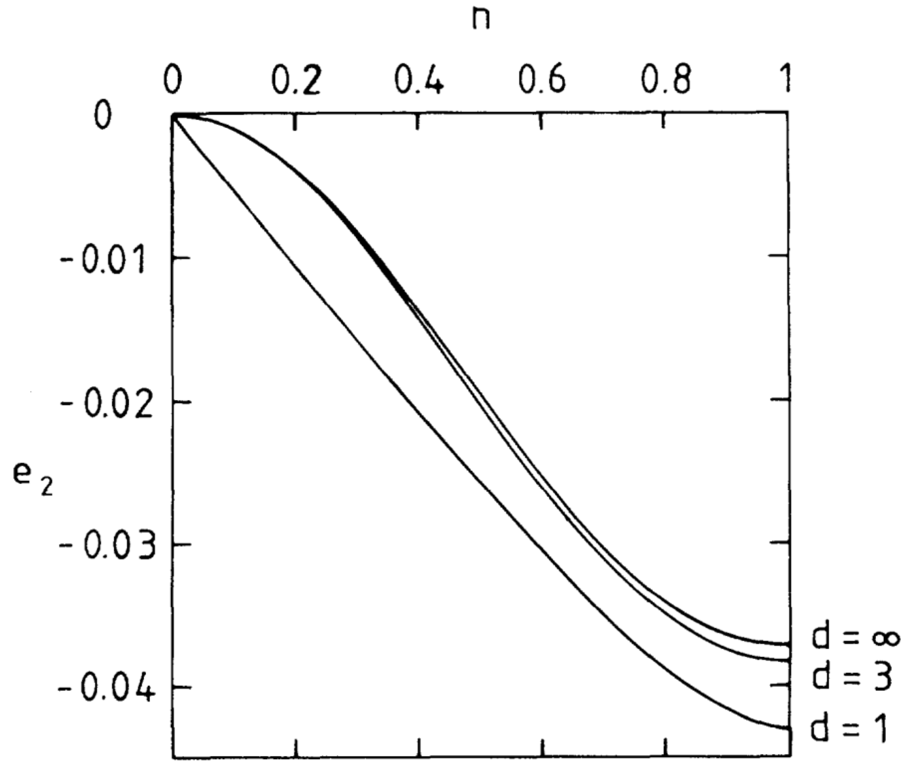

FIG. 2: Second-order contribution to the correlation energy $e_2 \equiv E_2/\left[LU^2/|\bar{\epsilon_0}(\frac{1}{2},\frac{1}{2})|\right]$ versus density, for lattice dimensions $d = 1, 3$, and ∞. $\bar{\epsilon_0}(n_\uparrow, n_\downarrow)$ is the kinetic energy of the non interacting particles for arbitrary densities $n_\uparrow$, $n_\downarrow$. Reprinted figure with permission from Ref.[1].

Given $G_{lat,p}(i\omega_n)$ and $\Sigma_p(i\omega_n)$, we obtain the effective non-interacting Green's function of the Anderson model, $\mathcal{G}_{0,p}^{-1}(i\omega_n)$, using Eq. (49). In order to close the self-consistent loop, the most numerically challenging step remains to be executed: solve the Anderson model, i.e., calculate its Green's function, knowing $\mathcal{G}_{0,p}^{-1}(i\omega_n)$. This is an active reasearch area in itself, and various numerical schemes have been developed in recent years. As an example, the so-called hybridization expansion algorithm[20] allows one to determine the Green's function for the Anderson model in Matsubara frequencies, i.e. solves the following model

$$\sum_\sigma \int_0^\beta d\tau \left(- \int_0^\beta d\tau' \; \phi_{0\sigma}^* \left[\mathcal{G}_0^{-1}(\tau')\delta(\tau-\tau')\right]\phi_{0\sigma} \right) + H_U(\phi_{0\uparrow}^*, \phi_{0\downarrow}^*, \phi_{0\uparrow}, \phi_{0\downarrow}). \tag{53}$$

Equipped with this tool, we obtain the impurity Green's function $G_p(i\omega_n)$ and can use Dyson's equation to obtain a new estimate for the self-energy of the impurity:

$$\Sigma_{p+1}(i\omega_n) = \mathcal{G}_{0,p}^{-1}(i\omega_n) - G_p(i\omega_n). \tag{54}$$

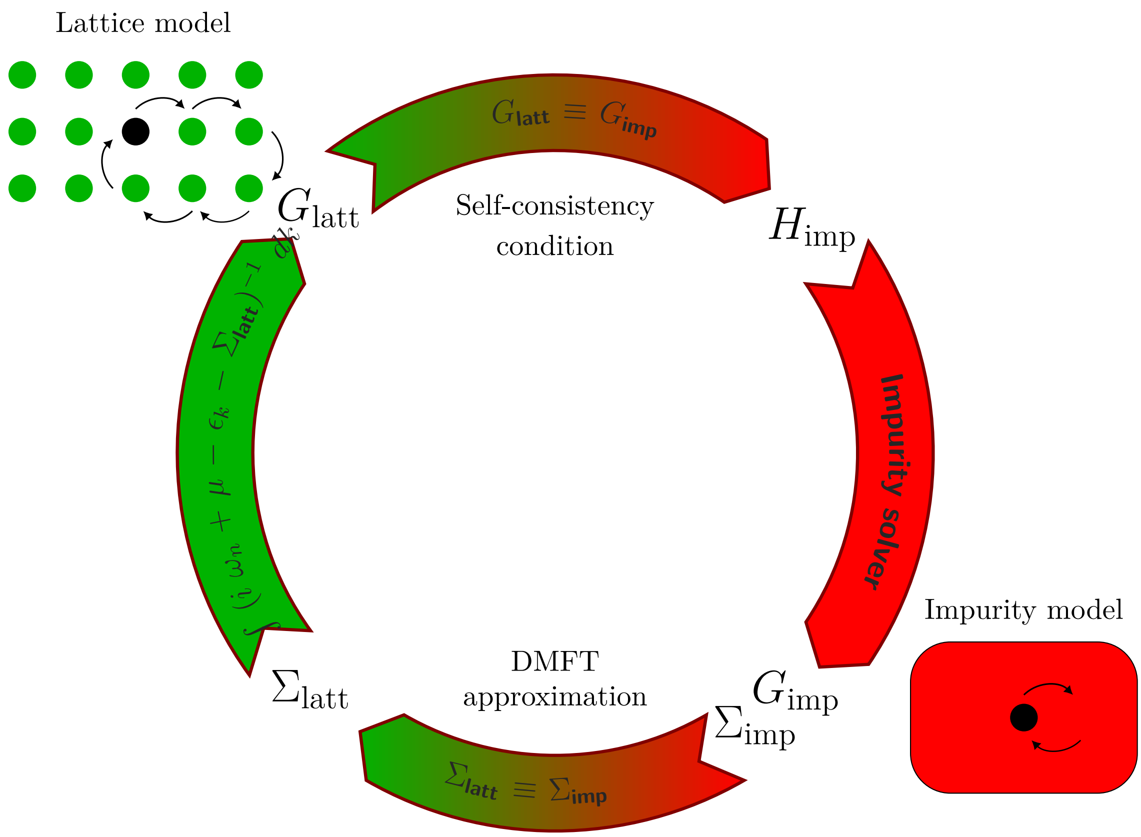

FIG. 3: The DMFT self-consistency loop. On the right-hand side, the system is considered from the point of view of an impurity in a bath of conduction electrons whose characteristics are known. On the left-hand side, the problem is viewed as a lattice whose self-energy is known.

This process is illustrated in Fig. 3. It can be iterated until it reaches convergence, i.e. until $\|\Sigma_p - \Sigma_{p+1}\| < \epsilon$, where $\|\ldots\|$ denotes a suitably chosen norm over functions, and ϵ is a suitably chosen convergence criterion. Experience has shown that this convergence is remarkably robust. Far away from phase transitions, convergence is quick and can be achieved in a few tens of iterations.

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