13 Quantum Cluster Methods: CPT and CDMFT

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1 Introduction

1.1 The Hubbard model and Green functions

Quantum cluster methods are schemes used to obtain approximate solutions of models of interacting electrons on a lattice. These models are used to describe classes of materials, such as high-temperature superconductors, in which electron-electron interactions are strong and for which the – otherwise successful – ideas behind Fermi liquid theory do not seem useful. The prototype of such models is the one-band Hubbard model. Other lectures in this volume offer extensive background material on this model; let us nevertheless write its Hamiltonian once more, in order to establish notation:

$$H = H_0 + H_1 \qquad \qquad H_0 = \sum_{\boldsymbol{r}, \boldsymbol{r}', \sigma} t_{\boldsymbol{r}\boldsymbol{r}'} c_{\boldsymbol{r}\sigma}^{\dagger} c_{\boldsymbol{r}'\sigma} \qquad \qquad H_1 = U \sum_{\boldsymbol{r}} n_{\boldsymbol{r}\uparrow} n_{\boldsymbol{r}\downarrow} \qquad (1)$$

 H_0 is the one-body term, which defines the band structure of the model, whereas H_1 is the electron-electron interaction. Sites of the Bravais lattice are indexed by the associated lattice vectors \boldsymbol{r} . The operator $c_{r\sigma}$ destroys an electron in a Wannier orbital of spin projection σ centered at site \boldsymbol{r} . The number of electrons in that orbital is $n_{r\sigma} = c_{r\sigma}^{\dagger} c_{r\sigma}$ and the total number of electrons at that site is $n_r = n_{r\uparrow} + n_{r\downarrow}$. The Hermitian hopping matrix $t_{rr'}$ defines the band structure; its Fourier transform is the dispersion relation $\varepsilon(\boldsymbol{k})$:

$$t_{\boldsymbol{r}\boldsymbol{r}'} = \frac{1}{N} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} \varepsilon(\boldsymbol{k}) .$$
⁽²⁾

Periodic boundary conditions are used, and the number N of sites in the system is assumed to be very large. For convenience, we will include the chemical potential in the one-body part H_0 , i.e., $t_{rr} = -\mu$.

A more general model might include more than one band; a band index n is then needed to label one-body states: $(\mathbf{r}, \sigma) \rightarrow (n, \mathbf{r}, \sigma)$. The hopping matrix then becomes a more general hybridization matrix $t_{n\mathbf{r},n'\mathbf{r}'}$, and there may be inter-band Coulomb interactions, Hund's couplings, and so on. The methods presented in this chapter may also be applied to such cases, but we will base our arguments on model (1), possibly augmented by longer-range Coulomb interactions (Sect. 6). In order to keep the discussion as general as possible, we will introduce a general index $\alpha = (n, \mathbf{r}, \sigma)$ that is a composite of position, spin and band indices. The first letters of the Greek alphabet $(\alpha, \beta, ...)$ will be used for that purpose.

The one-particle Green function A complete solution to model (1) at zero temperature would be provided by the many-body ground state $|\Omega\rangle$. Such an object, even if it were known, would be too unwieldy and would contain much more information than what is necessary to make useful predictions. We will instead seek approximate solutions for the one-particle Green function, defined at zero-temperature and as a function of complex frequency z as

$$G_{\alpha\beta}(z) = \left\langle \Omega \left| c_{\alpha} \frac{1}{z - H + E_0} c_{\beta}^{\dagger} \right| \Omega \right\rangle + \left\langle \Omega \left| c_{\beta}^{\dagger} \frac{1}{z + H - E_0} c_{\alpha} \right| \Omega \right\rangle, \tag{3}$$

where E_0 is the ground state energy associated with the Hamiltonian H, which, let us not forget, includes the chemical potential. $G_{\alpha\beta}(z)$ contains dynamical information about one-particle excitations, such as the spectral weight measured in ARPES experiments. We will generally use a boldface matrix notation (G) for quantities carrying two one-body indices ($G_{\alpha\beta}$).

A finite-temperature expression for the Green function (3) is obtained by simply replacing the ground state expectation value by a thermal average. Practical computations at finite temperature are mostly done using Monte Carlo methods, which rely on the path integral formalism and are performed as a function of imaginary time, not directly as a function of real frequencies. In the limited scope of this chapter, we will confine ourselves to the zero-temperature formalism.

Green function in the time domain The expression (3) may be unfamiliar to those used to a definition of the Green function in the time domain. Let us just mention the connection. We define the spectral function in the time domain and its Fourier transform as

$$A_{\alpha\beta}(t) = \langle \{c_{\alpha}(t), c_{\beta}^{\dagger}(0)\} \rangle \qquad \qquad A_{\alpha\beta}(\omega) = \int_{-\infty}^{\infty} dt \ e^{i\omega t} A_{\alpha\beta}(t) \tag{4}$$

where $\{\cdot, \cdot\}$ is the anticommutator and z is a complex frequency. The time dependence is defined in the Heisenberg picture, i.e., $c_{\alpha}(t) = e^{iHt}c_{\alpha}(0)e^{-iHt}$, where H includes the chemical potential. Then it can be shown that the Green function is related to $A_{\alpha\beta}(z)$ by

$$G_{\alpha\beta}(z) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A_{\alpha\beta}(\omega)}{z - \omega} \quad .$$
(5)

The retarded Green function $G^R_{\alpha\beta}(t)$ is defined in the time domain as

$$G^{R}_{\alpha\beta}(t) = -i\Theta(t)\langle\{c_{\alpha}(t), c^{\dagger}_{\beta}(0)\}\rangle = -i\Theta(t)A_{\alpha\beta}(t)$$
(6)

where $\Theta(t)$ is the Heaviside step function. Since the Fourier transform of the latter is

$$\mathcal{F}(\Theta)(\omega) = \int_0^\infty dt \ e^{i\omega t} = \frac{1}{\omega + i0^+} , \qquad (7)$$

a simple convolution shows that

$$G^{R}_{\alpha\beta}(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A_{\alpha\beta}(\omega')}{\omega - \omega' + i0^{+}} = G_{\alpha\beta}(\omega + i0^{+}) \quad .$$
(8)

In fact, this connection can be established easily from the spectral representation, introduced next.

Spectral representation Let $\{|r\rangle\}$ be a complete set of eigenstates of H with one particle *more* than the ground state, where r is a positive integer label. Likewise, let us use negative integer labels to denote eigenstates of H with one particle *less* than the ground state. Then, by inserting completeness relations,

$$G_{\alpha\beta}(z) = \sum_{r>0} \langle \Omega | c_{\alpha} | r \rangle \frac{1}{z - E_r + E_0} \langle r | c_{\beta}^{\dagger} | \Omega \rangle + \sum_{r<0} \langle \Omega | c_{\beta}^{\dagger} | r \rangle \frac{1}{z + E_r - E_0} \langle r | c_{\alpha} | \Omega \rangle .$$
(9)

By setting

$$Q_{\alpha r} = \begin{cases} \langle \Omega | c_{\alpha} | r \rangle & (r > 0) \\ \langle r | c_{\alpha} | \Omega \rangle & (r < 0) \end{cases} \quad \text{and} \quad \omega_r = \begin{cases} E_r - E_0 & (r > 0) \\ E_0 - E_r & (r < 0) \end{cases}$$
(10)

we write

$$G_{\alpha\beta}(z) = \sum_{r} \frac{Q_{\alpha r} Q_{\beta r}^*}{z - \omega_r} \ . \tag{11}$$

This shows how the Green function is a sum over poles located at $\omega_r \in \mathbb{R}$, with residues that are products of overlaps of the ground state with energy eigenstates with one more ($\omega_r > 0$) or one less ($\omega_r < 0$) particle. The sum of residues is normalized to the unit matrix, as can be seen from the anticommutation relations:

$$\sum_{r} Q_{\alpha r} Q_{\beta r}^{*} = \sum_{r>0} \langle \Omega | c_{\alpha} | r \rangle \langle r | c_{\beta}^{\dagger} | \Omega \rangle + \sum_{r<0} \langle \Omega | c_{\beta}^{\dagger} | r \rangle \langle r | c_{\alpha} | \Omega \rangle$$

= $\langle \Omega | \left(c_{\alpha} c_{\beta}^{\dagger} + c_{\beta}^{\dagger} c_{\alpha} \right) | \Omega \rangle = \delta_{\alpha\beta} .$ (12)

Thus, in the high-frequency limit, $G(z \to \infty) = 1/z$ (1 stands for the unit matrix). The same procedure applied to the spectral function (4) leads easily to

$$A_{\alpha\beta}(\omega) = 2\pi \sum_{r} Q_{\alpha r} Q_{\beta r}^* \,\delta(\omega - \omega_r)\,,\tag{13}$$

and this demonstrates the connection (5) between $A_{\alpha\beta}(\omega)$ and $G_{\alpha\beta}(z)$. The property (12) amounts to saying that $A_{\alpha\alpha}(\omega)$ is a probability density:

$$A_{\alpha\alpha}(\omega) = 2\pi \sum_{r} |Q_{\alpha r}|^2 \,\delta(\omega - \omega_r) \qquad \qquad \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_{\alpha\alpha}(\omega) = 1 \tag{14}$$

The identity

$$-\frac{1}{\pi}\operatorname{Im}\frac{1}{\omega+i0^{+}} = \delta(\omega) \tag{15}$$

implies that

$$A_{\alpha\alpha}(\omega) = -2 \operatorname{Im} G_{\alpha\alpha}(\omega + i0^{+}) \quad . \tag{16}$$

From the definition of $Q_{\alpha r}$, one sees that $A_{\alpha\alpha}(\omega)$ is the probability density for an electron added or removed from the ground state in the one-particle state α to have an energy ω . The density of states $\rho(\omega)$ is simply the trace

$$\rho(\omega) = \frac{1}{N} \sum_{\alpha} A_{\alpha\alpha}(\omega) = -\frac{2}{N} \operatorname{Im} \operatorname{tr} \boldsymbol{G}(\omega + i0^{+}) .$$
(17)

Self-energy In the absence of interactions $(H_1 = 0)$ the Hamiltonian reduces to $H_0 = \sum_{\alpha,\beta} t_{\alpha\beta} c^{\dagger}_{\alpha} c_{\beta}$. Since the matrix t is Hermitian, there exists a basis $\{|\ell\rangle\}$ of one-body states that diagonalizes it: $H_0 = \sum_{\ell} \varepsilon_{\ell} c^{\dagger}_{\ell} c_{\ell}$. The ground state is then the filled Fermi sea:

$$|\Omega\rangle = \prod_{\varepsilon_{\ell} < 0} c_{\ell}^{\dagger} |0\rangle \tag{18}$$

and one-particle excited states are $c_{\ell}^{\dagger} | \Omega \rangle$ ($\varepsilon_{\ell} > 0$) with $E_{\ell} - E_0 = \varepsilon_{\ell}$ and $c_{\ell} | \Omega \rangle$ ($\varepsilon_{\ell} < 0$) with $E_{\ell} - E_0 = -\varepsilon_{\ell}$. The spectral representation is in that case extremely simple and the matrix $G = G_0$ is diagonal:

$$G_{0,\ell\ell'}(z) = \frac{\delta_{\ell\ell'}}{z - \varepsilon_{\ell}}.$$
(19)

In any other basis of one-body states in which t is not diagonal, the expression is simply

$$\boldsymbol{G}_0(z) = \frac{1}{z - \boldsymbol{t}} \,. \tag{20}$$

In the presence of interactions, the Green function takes the following general form:

$$\boldsymbol{G}(z) = \frac{1}{z - \boldsymbol{t} - \boldsymbol{\Sigma}(z)},$$
(21)

where all the information related to H_1 is buried within the self-energy $\Sigma(z)$. The relation (21), called *Dyson's equation*, may be regarded as a definition of the self-energy. It can be shown that the self-energy has a spectral representation similar to that of the Green function:

$$\Sigma_{\alpha\beta}(z) = \Sigma_{\alpha\beta}^{\infty} + \sum_{r} \frac{S_{\alpha r} S_{\beta r}^{*}}{z - \sigma_{r}} , \qquad (22)$$

where the σ_r are poles located on the real axis (they are zeros of the Green function). By contrast with the Green function, the self-energy may have a frequency-independent piece $\sum_{\alpha\beta}^{\infty}$, which has the same effect as a hopping term; in fact, within the Hartree-Fock approximation, this is the only piece of the self-energy that survives.

Averages of one-body operators Many physical observables are one-body operators, of the form

$$\mathcal{O} = \sum_{\alpha,\beta} s_{\alpha\beta} c^{\dagger}_{\alpha} c_{\beta} \,. \tag{23}$$

The ground-state expectation value of such operators can be computed from the Green function $G_{\alpha\beta}(z)$. Let us explain how.

From the spectral representation (11) of the Green function, we see that $\langle c_{\alpha}^{\dagger} c_{\beta} \rangle$ is given by the integral of the Green function along a contour $C_{<}$ surrounding the negative real axis counterclockwise:

$$\langle c_{\alpha}^{\dagger} c_{\beta} \rangle = \int_{C_{<}} \frac{\mathrm{d}z}{2\pi i} G_{\beta\alpha}(z) \,.$$
(24)

Therefore the expectation value we are looking for is

$$\bar{\mathcal{O}} = \frac{1}{N} \sum_{\alpha,\beta} s_{\alpha\beta} \left\langle c_{\alpha}^{\dagger} c_{\beta} \right\rangle = \frac{1}{N} \int_{C_{<}} \frac{\mathrm{d}z}{2\pi i} \operatorname{tr} \left[\boldsymbol{s} \, \boldsymbol{G}(z) \right]$$
(25)

(we divide by N to find an intensive quantity). The trace includes a sum over lattice sites, spin and band indices.

The contour $C_{<}$ can be taken as the imaginary axis (from -iR to iR), plus the left semi-circle of radius R. Since $G(z) \rightarrow 1/z$ as $z \rightarrow \infty$, the semi-circular part will contribute, but this



Fig. 1: *Tiling of the triangular lattice by* 6*-site triangular clusters. The super-cells are delimited by dashed lines.*

contribution may be canceled by subtracting from G(z) a term like 1/(z-p), with p > 0: the added term does not contribute to the integral, since its only pole lies outside the contour, yet it cancels the dominant z^{-1} behavior as $z \to \infty$, leaving a contribution that vanishes on the semi-circle as $R \to \infty$. We are left with

$$\bar{\mathcal{O}} = \frac{1}{N} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \left\{ \operatorname{tr} \left[\boldsymbol{s} \, \boldsymbol{G}(i\omega) \right] - \frac{\mathrm{tr} \, \boldsymbol{s}}{i\omega - p} \right\} \,.$$
(26)

If the operator \mathcal{O} is Hermitian, so is the matrix s. By virtue of the property $G(z)^{\dagger} = G(z^*)$, easily seen from (11), we have $\operatorname{tr} [s G(-i\omega)] = \operatorname{tr} [s G(i\omega)]^*$; this implies that $\overline{\mathcal{O}}$ is real.

1.2 Clusters

How can we compute G(z) if the many-body ground state $|\Omega\rangle$ is not known? Quantum cluster methods provide an approximate solution by dividing the original system into smaller parts. The original lattice γ is tiled into small, manageable and disconnected clusters. For instance, the triangular lattice may be tiled by 6-site clusters, as illustrated in Fig. 1; in that case, two distinct clusters are included in each repeated unit, or *super-cell*. On a cluster labeled j, a Hamiltonian $H^{(j)}$ is defined, whose interaction part $H_1^{(j)}$ coincides with that of the original problem:

$$H_1 = \sum_j H_1^{(j)},$$
 (27)

but whose one-body part $H_0^{(j)}$ will depend on the particular quantum cluster method used. In order to stay general, we have left open the possibility that the cluster Hamiltonians $H^{(j)}$ are all different from one another, for instance because of a position-dependent potential added to the basic Hubbard model. However, in most cases, they will all be identical to one or a few clusters forming a repeated super-cell.

Each cluster's one-particle Green function $G^{(j)}(z)$ needs to be computed. Various numerical methods may be harnessed for this task. At zero temperature, exact diagonalization techniques

are generally used; this entails computing the many-body ground state $|\Omega^{(j)}\rangle$ of $H^{(j)}$ and applying the definition (3) to find $G^{(j)}$, as explained summarily in Sect. 3.

Then the self-energy $\Sigma^{(j)}(z)$ associated with $G^{(j)}(z)$ is extracted from Dyson's equation, and the following approximation for the lattice self-energy is assembled:

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}^{(1)} & 0 & \cdots & 0 \\ 0 & \boldsymbol{\Sigma}^{(2)} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \boldsymbol{\Sigma}^{(n)} \end{pmatrix}.$$
 (28)

This equation defines the basic assumption behind quantum cluster methods: the self-energy can be approximated by the direct sum of the self-energies of all clusters. The lattice Green function is then constructed from the Dyson equation (21). Note that in the simple case of a super-cell made of a single cluster, all self-energies $\Sigma^{(j)}$ are identical.

Many relevant physical properties of the model can be extracted from the one-particle Green function, as shown in Eq. (26), but not all. Other functions of interest relevant to experiments are the dynamical susceptibilities, where the creation and annihilation operators of Eq. (3) are replaced by one-body operators, such as the spin or electron densities. However, the methods described in this chapter will not provide us with approximate ways to compute these properties, beyond computing them within each cluster.

1.3 Cluster Perturbation Theory

The simplest of all quantum cluster methods is *Cluster Perturbation Theory* (CPT) [1,2]. In CPT, each cluster's one-body Hamiltonian $H_0^{(j)}$ is simply the restriction to the cluster of the full one-body Hamiltonian H_0 . If hopping terms connecting sites located on cluster *i* to those of cluster *j* are collected into a matrix $t^{(i,j)}$, then the full one-body matrix may be expressed as

$$\boldsymbol{t} = \begin{pmatrix} \boldsymbol{t}^{(1,1)} & \boldsymbol{t}^{(1,2)} & \cdots & \boldsymbol{t}^{(1,n)} \\ \boldsymbol{t}^{(2,1)} & \boldsymbol{t}^{(2,2)} & \cdots & \boldsymbol{t}^{(2,n)} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{t}^{(n,1)} & \boldsymbol{t}^{(n,2)} & \cdots & \boldsymbol{t}^{(n,n)} \end{pmatrix}$$
(29)

The one-body matrix defining $H_0^{(j)}$ in CPT is then simply the diagonal block $t^{(j,j)}$ and each cluster's interacting Green function obeys the relation

$$\boldsymbol{G}^{(j)^{-1}}(z) = z - \boldsymbol{t}^{(j,j)} - \boldsymbol{\Sigma}^{(j)}(z)$$
(30)

The basic approximation (28), when combined with Eqs (21) and (29), leads to the following formula for the approximate, or CPT, Green function:

$$\boldsymbol{G}_{\rm cpt}^{-1}(z) = \bigoplus_{j} \, \boldsymbol{G}^{(j)^{-1}}(z) - \boldsymbol{t}_{\rm ic} \,, \qquad (31)$$

where \oplus stands for the direct sum, and the matrix t_{ic} is obtained from t in Eq. (29) by removing all diagonal blocks; it is the inter-cluster hopping matrix.

One may collectively denote by H' the sum of cluster Hamiltonians and by G' the direct sum of cluster Green functions:

$$H' = \sum_{j} H^{(j)} \qquad \qquad \mathbf{G}'(z) = \bigoplus_{j} \mathbf{G}^{(j)}(z) \tag{32}$$

We may then write simpler-looking formulas:

$$H = H' + \sum_{\alpha,\beta} (t_{\rm ic})_{\alpha\beta} c^{\dagger}_{\alpha} c_{\beta}$$
(33)

$$\boldsymbol{G}_{\rm cpt}^{-1}(z) = \boldsymbol{G}'^{-1}(z) - \boldsymbol{t}_{\rm ic}$$
(34)

Cluster Perturbation Theory is called this way because it can be derived by treating the second term of Eq. (33) as a perturbation on H'. It can be shown that, at lowest order in t_{ic} , the Green function is indeed given by Eq. (34) [2, 3].

Cluster Perturbation Theory has the following characteristics:

- 1. Although it is derived using strong-coupling perturbation theory, it is exact in the $U \rightarrow 0$ limit, since the self-energy disappears in that case.
- 2. It is also exact in the strong-coupling limit $t_{rr'}/U \rightarrow 0$.
- 3. It provides an approximate lattice Green function for arbitrary wave-vectors, as explained in Sect. 2.2 below, hence its usefulness in comparing with ARPES data.
- 4. Although formulated as a lowest-order result of strong-coupling perturbation theory, it is not controlled by including higher-order terms in that perturbation expansion this would be extremely difficult but rather by increasing the cluster size.
- 5. It cannot describe broken-symmetry states. This is accomplished by more sophisticated approaches like the Variational Cluster Approximation (VCA) and Cluster Dynamical Mean Field Theory (CDMFT), which can both be viewed as extensions or refinements of CPT. But even in these approaches, formula (34) still applies. The difference lies in the use of different cluster Hamiltonians $H_0^{(j)}$ and therefore different cluster Green functions $G^{(j)}$.

2 Periodic systems

2.1 Cluster kinematics

Typically, the clusters that 'tile' the lattice are repeated: one or a few of them form a repeated *super-cell*, like the two 6-site clusters of Fig. 1. Mathematically, this corresponds to introducing a super-lattice Γ , whose sites form a subset of the original lattice γ that will be labeled by the positions \tilde{r} . This super-lattice is generated by basis vectors $\{e_1, e_2, e_3\}$: every site \tilde{r} of the super-lattice may be expressed as an integer combination of these basis vectors. Associated with each site of Γ is a super-cell containing L sites. The super-cell is made of one cluster, or



Fig. 2: Left panel: Tiling of the square lattice with identical ten-site clusters (L = 10). The vectors $e_{1,2}$ define a super-lattice of clusters. Right panel: the corresponding Brillouin zones. The reduced Brillouin zone (tilted black square) is associated with the super-lattice and L copies of it can be fitted within the original Brillouin zone (large square).

sometimes of a few clusters, as in Fig. 1. Note that the shape of these clusters is not uniquely determined by the super-lattice structure. The sites within each super-cell will be labeled by their vector position (in capitals): \mathbf{R} , \mathbf{R}' , etc. Each site \mathbf{r} of the original lattice γ can therefore be expressed uniquely as $\mathbf{r} = \tilde{\mathbf{r}} + \mathbf{R}$.

The Brillouin zone of the original lattice, denoted BZ_{γ} , contains L points belonging to the reciprocal super-lattice Γ^* . The Brillouin zone of the super-lattice BZ_{Γ} has a volume L times smaller than that of BZ_{γ} . Any wave-vector k of the original Brillouin zone can be uniquely expressed as $k = K + \tilde{k}$, where K belongs both to the reciprocal super-lattice and to BZ_{γ} , and \tilde{k} belongs to BZ_{Γ} (see Fig. 2).

The passage between momentum space and real space, via discrete Fourier transforms can be done either directly $(r \leftrightarrow k)$ or independently for cluster and super-lattice sites $(\tilde{r} \leftrightarrow \tilde{k}$ and $R \leftrightarrow K$). This can be encoded into unitary matrices U^{γ} , U^{Γ} and U^{c} defined as follows:

$$U_{\boldsymbol{k},\boldsymbol{r}}^{\gamma} = \frac{1}{\sqrt{N}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} , \quad U_{\boldsymbol{\tilde{k}}\boldsymbol{\tilde{r}}}^{\Gamma} = \sqrt{\frac{L}{N}} e^{-i\boldsymbol{\tilde{k}}\cdot\boldsymbol{\tilde{r}}} , \quad U_{\boldsymbol{K},\boldsymbol{R}}^{c} = \frac{1}{\sqrt{L}} e^{-i\boldsymbol{K}\cdot\boldsymbol{R}} , \quad (35)$$

where again N is the (large) number of sites in the original lattice γ , which can be treated with periodic boundary conditions at the edges. The matrix U^{γ} is of order N, U^{Γ} is of order N/Land U^{c} of order L.

The discrete Fourier transforms on a generic one-index quantity f are then

$$f(\boldsymbol{k}) = \sum_{\boldsymbol{r}} U_{\boldsymbol{k},\boldsymbol{r}}^{\gamma} f_{\boldsymbol{r}} \quad , \quad f(\tilde{\boldsymbol{k}}) = \sum_{\tilde{\boldsymbol{r}}} U_{\tilde{\boldsymbol{k}},\tilde{\boldsymbol{r}}}^{\Gamma} f_{\tilde{\boldsymbol{r}}} \quad , \quad f_{\boldsymbol{K}} = \sum_{\boldsymbol{R}} U_{\boldsymbol{K},\boldsymbol{R}}^{c} f_{\boldsymbol{R}} \tag{36}$$

or, in reverse,

$$f_{\boldsymbol{r}} = \sum_{\boldsymbol{k}} U_{\boldsymbol{k},\boldsymbol{r}}^{\gamma*} f(\boldsymbol{k}) \quad , \quad f_{\tilde{\boldsymbol{r}}} = \sum_{\tilde{\boldsymbol{k}}} U_{\tilde{\boldsymbol{k}},\tilde{\boldsymbol{r}}}^{\Gamma*} f(\tilde{\boldsymbol{k}}) \quad , \quad f_{\boldsymbol{R}} = \sum_{\boldsymbol{K}} U_{\boldsymbol{K},\boldsymbol{R}}^{c*} f_{\boldsymbol{K}}$$
(37)

These discrete Fourier transforms close by virtue of the following identities

$$\frac{1}{N}\sum_{\boldsymbol{k}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \delta_{\boldsymbol{r}} \qquad \qquad \frac{L}{N}\sum_{\tilde{\boldsymbol{k}}}e^{i\tilde{\boldsymbol{k}}\cdot\tilde{\boldsymbol{r}}} = \delta_{\tilde{\boldsymbol{r}}} \qquad \qquad \frac{1}{L}\sum_{\boldsymbol{K}}e^{i\boldsymbol{K}\cdot\boldsymbol{R}} = \delta_{\boldsymbol{R}} \quad (38)$$

$$\frac{1}{N}\sum_{\boldsymbol{r}}e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} = \delta_{\boldsymbol{k}} \qquad \qquad \frac{L}{N}\sum_{\tilde{\boldsymbol{r}}}e^{-i\tilde{\boldsymbol{k}}\cdot\tilde{\boldsymbol{r}}} = \delta_{\tilde{\boldsymbol{k}}} \qquad \qquad \frac{1}{L}\sum_{\boldsymbol{R}}e^{-i\boldsymbol{K}\cdot\boldsymbol{R}} = \delta_{\boldsymbol{K}} \quad (39)$$

where δ_r is the usual Kronecker delta, used for all labels (since they are all discrete):

$$\delta_{\alpha} = \begin{cases} 1 & \text{if } \alpha = 0 \\ 0 & \text{otherwise} \end{cases} \qquad \delta_{\alpha\beta} \equiv \delta_{\alpha-\beta} , \qquad (40)$$

It is implicit that the Kronecker deltas are periodic, i.e., that $\delta_{\tilde{k}} = \delta_{\tilde{k}+K}$, for instance.¹ A one-index quantity like the destruction operator $c_r = c_{\tilde{r}+R}$ can be represented in a variety of ways through partial Fourier transforms:

$$c_{\boldsymbol{R}}(\tilde{\boldsymbol{k}}) = \sum_{\tilde{\boldsymbol{r}}} U_{\tilde{\boldsymbol{k}}\tilde{\boldsymbol{r}}}^{\Gamma} c_{\tilde{\boldsymbol{r}}+\boldsymbol{R}} \qquad c_{\boldsymbol{K}}(\tilde{\boldsymbol{k}}) = \sum_{\tilde{\boldsymbol{r}},\boldsymbol{R}} U_{\tilde{\boldsymbol{k}}\tilde{\boldsymbol{r}}}^{\Gamma} U_{\boldsymbol{K}\boldsymbol{R}}^{c} c_{\tilde{\boldsymbol{r}}+\boldsymbol{R}}$$

$$c_{\tilde{\boldsymbol{r}},\boldsymbol{K}} = \sum_{\boldsymbol{R}} U_{\boldsymbol{K}\boldsymbol{R}}^{c} c_{\tilde{\boldsymbol{r}}+\boldsymbol{R}} \qquad c(\boldsymbol{k}) = \sum_{\boldsymbol{r}} U_{\boldsymbol{k}\boldsymbol{r}}^{\gamma} c_{\boldsymbol{r}}$$

$$(41)$$

Note that

$$\boldsymbol{k} \cdot \boldsymbol{r} = (\tilde{\boldsymbol{k}} + \boldsymbol{K}) \cdot (\tilde{\boldsymbol{r}} + \boldsymbol{R}) = \tilde{\boldsymbol{k}} \cdot \tilde{\boldsymbol{r}} + \boldsymbol{K} \cdot \boldsymbol{R} + \tilde{\boldsymbol{k}} \cdot \boldsymbol{R} + \boldsymbol{K} \cdot \tilde{\boldsymbol{r}} .$$
(42)

By definition, the last term is a multiple of 2π (K is an element of the reciprocal lattice γ^*). Therefore the two representations c(k) and $c_K(\tilde{k})$ are not identical, since the phases involved in (41), $k \cdot r$ and $\tilde{k} \cdot \tilde{r} + K \cdot R$, differ by $\tilde{k} \cdot R$. These two representations are obtained respectively by applying the unitary matrices $S \equiv U^{\Gamma} \otimes U^{c}$ and U^{γ} on the r basis, and these two operations are different since the $N \times N$ matrix $\Lambda \equiv U^{\gamma}S^{-1}$ is not trivial:

$$\Lambda_{\boldsymbol{k}\boldsymbol{k}'} = \delta_{\tilde{\boldsymbol{k}}\tilde{\boldsymbol{k}}'} \Lambda^{c}_{\boldsymbol{K}\boldsymbol{K}'}(\tilde{\boldsymbol{k}}) \quad \text{where} \quad \Lambda^{c}_{\boldsymbol{K}\boldsymbol{K}'}(\tilde{\boldsymbol{k}}) = \frac{1}{L} \sum_{\boldsymbol{R}} e^{-i\boldsymbol{R}\cdot(\tilde{\boldsymbol{k}}+\boldsymbol{K}-\boldsymbol{K}')} \,. \tag{43}$$

The matrix $\Lambda^{c}(\tilde{k})$ is $L \times L$ and connects the (K, \tilde{k}) basis to the $k = \tilde{k} + K$ basis:

$$c(\tilde{\boldsymbol{k}} + \boldsymbol{K}) = \sum_{\boldsymbol{K}'} \Lambda^{c}_{\boldsymbol{K}\boldsymbol{K}'}(\tilde{\boldsymbol{k}}) c_{\boldsymbol{K}'}(\tilde{\boldsymbol{k}}) .$$
(44)

A two-index quantity like the hopping matrix $t_{rr'}$ or the Green function $G_{rr'}$ has a number of different representations. The first index transforms like c_r and the second like $c_{r'}^{\dagger}$. For instance,

$$t(\boldsymbol{k}, \boldsymbol{k}') = \sum_{\boldsymbol{r}, \boldsymbol{r}'} U_{\boldsymbol{k}\boldsymbol{r}}^{\gamma} U_{\boldsymbol{k}'\boldsymbol{r}'}^{\gamma*} t_{\boldsymbol{r}\boldsymbol{r}'} .$$
(45)

¹Such periodic Kronecker deltas are sometimes called Laue functions.

Due to translation invariance on the lattice, this matrix is diagonal when expressed in momentum space: $t(\mathbf{k}, \mathbf{k}') = \varepsilon(\mathbf{k}) \, \delta_{\mathbf{k},\mathbf{k}'}, \, \varepsilon(\mathbf{k})$ being the dispersion relation (2). However, in practice we most often use the mixed representation

$$t_{\boldsymbol{R}\boldsymbol{R}'}(\tilde{\boldsymbol{k}}) = \sum_{\tilde{\boldsymbol{r}}} e^{i\tilde{\boldsymbol{k}}\cdot\tilde{\boldsymbol{r}}} t_{\boldsymbol{r}\boldsymbol{r}'} \text{ where } \boldsymbol{r} = \boldsymbol{R} \text{ and } \boldsymbol{r}' = \tilde{\boldsymbol{r}} + \boldsymbol{R}'.$$
 (46)

For instance, if we tile the one-dimensional lattice with clusters of length L = 2, the nearestneighbor hopping matrix, corresponding to the dispersion relation $\varepsilon(k) = -2t \cos(k) - \mu$, has the following mixed representation:

$$\mathbf{t}(\tilde{k}) = -\begin{pmatrix} \mu & t(1 + e^{-2i\tilde{k}}) \\ t(1 + e^{2i\tilde{k}}) & \mu \end{pmatrix} .$$
(47)

Finally, let us point out that the space E of one-electron states is larger than the space of lattice sites γ , as it also includes spin and maybe band degrees of freedom, which form a set B. We could therefore write $E = \gamma \otimes B$. The transformation matrices defined above $(U^{\gamma}, U^{\Gamma} \text{ and } U^{c})$ should, as necessary, be understood as tensor products $(U^{\gamma} \otimes 1, U^{\Gamma} \otimes 1 \text{ and } U^{c} \otimes 1)$ acting trivially in B. This should be clear from the context. The total number of degrees of freedom in the super-cell is therefore an integer multiple of L, which we shall denote by M_{sc} .

2.2 The CPT Green function and periodization

The most convenient representation for periodic systems is the (\mathbf{R}, \mathbf{k}) scheme, which uses realspace indices in the super-cell and reduced wave-vectors. Because of translational invariance, the inter-cluster hopping matrix of Eq. (34) is diagonal in $\mathbf{\tilde{k}}$ and \mathbf{t}_{ic} , becoming effectively a M_{sc} -dimensional, $\mathbf{\tilde{k}}$ -dependent matrix $\mathbf{t}_{ic}(\mathbf{\tilde{k}})$. If the super-cell contains more than one cluster, like the example of Fig. 1, the matrix \mathbf{t}_{ic} also contains $\mathbf{\tilde{k}}$ -independent terms from the hopping terms between those. Likewise, the restriction of \mathbf{G}' (32) to the super-cell is M_{sc} -dimensional, the same for all super-cells, and therefore $\mathbf{\tilde{k}}$ -independent. We will also denote it by \mathbf{G}' , even though this is a slight abuse of notation. Therefore, Eq. (34) becomes

$$\boldsymbol{G}_{\text{cpt}}^{-1}(z, \tilde{\boldsymbol{k}}) = \boldsymbol{G}'^{-1}(z) - \boldsymbol{t}_{\text{ic}}(\tilde{\boldsymbol{k}})$$
(48)

In that relation, all matrices are of size M_{sc} . The super-cell Green function G' is either a single cluster Green function $G^{(j)}$, directly computed from the impurity solver, or a direct sum of the cluster Green functions making up the super-cell.

Relation (48) is the most convenient way to compute the CPT Green function. The cluster self-energies do not need to be extracted explicitly.

A supplemental ingredient of CPT is the *periodization* formula, which provides a fully *k*-dependent Green function out of the mixed representation $G_{RR'}(\tilde{k}, z)$. It was proposed in Ref. [2] to define the following *periodized* Green function:²

$$G_{\text{per.}}(\boldsymbol{k}, z) = \frac{1}{L} \sum_{\boldsymbol{R}, \boldsymbol{R}'} e^{-i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} G_{\boldsymbol{R}\boldsymbol{R}'}(\tilde{\boldsymbol{k}}, z) .$$
(49)

²In the following the spin and band indices are muted: the left hand side is still a matrix in those indices, but we will focus here on the spatial and wave-vector indices only, in order to lighten the notation.

Let us explain. Treating intra-cluster and inter-cluster hopping terms differently breaks the original translational symmetry of the model: The Green function (48) is not translationally invariant on the original lattice γ . This means that it is not diagonal when expressed in the k-scheme, i.e., $G(k, k') \neq 0$ if $k \neq k'$. However, because of the residual super-lattice translational invariance, k' and k must correspond to the same \tilde{k} and differ by an element of the reciprocal super-lattice: k' = k + K. Thus, in the (K, \tilde{k}) basis, the matrix G has the following form:

$$G_{\boldsymbol{K}\boldsymbol{K}'}(\tilde{\boldsymbol{k}},z) = \frac{1}{L} \sum_{\boldsymbol{R},\boldsymbol{R}'} e^{-i(\boldsymbol{K}\cdot\boldsymbol{R}-\boldsymbol{K}'\cdot\boldsymbol{R}')} G_{\boldsymbol{R}\boldsymbol{R}'}(\tilde{\boldsymbol{k}},z) .$$
(50)

Since an element of the reduced Brillouin zone is defined up to a vector belonging to the reciprocal super-lattice Γ^* , one may replace \tilde{k} by k in $G_{RR'}(\tilde{k}, z)$, i.e., $G_{RR'}(\tilde{k}, z) = G_{RR'}(\tilde{k}+K, z)$. This form can be further converted to the full wave-vector basis ($k = K + \tilde{k}$) by use of the unitary matrix Λ^c of Eq (43):

$$G(\tilde{\mathbf{k}} + \mathbf{K}, \tilde{\mathbf{k}} + \mathbf{K}') = \left(\mathbf{\Lambda}^{c}(\tilde{\mathbf{k}}) \mathbf{G} \mathbf{\Lambda}^{c\dagger}(\tilde{\mathbf{k}})\right)_{\mathbf{K}\mathbf{K}'}$$

$$= \frac{1}{L^{2}} \sum_{\mathbf{R}, \mathbf{R}', \mathbf{K}_{1}, \mathbf{K}'_{1}} e^{-i(\tilde{\mathbf{k}} + \mathbf{K} - \mathbf{K}_{1}) \cdot \mathbf{R}} e^{i(\tilde{\mathbf{k}} + \mathbf{K}' - \mathbf{K}'_{1}) \cdot \mathbf{R}'} G_{\mathbf{K}_{1}\mathbf{K}'_{1}}$$

$$= \frac{1}{L} \sum_{\mathbf{R}, \mathbf{R}'} e^{-i(\tilde{\mathbf{k}} + \mathbf{K}) \cdot \mathbf{R}} e^{i(\tilde{\mathbf{k}} + \mathbf{K}') \cdot \mathbf{R}'} G_{\mathbf{R}\mathbf{R}'}(\tilde{\mathbf{k}}, z) .$$
(51)

The periodization formula (49) amounts to picking the diagonal piece of the Green function $(\mathbf{K} = \mathbf{K}', \text{ or } \mathbf{k} = \mathbf{k}')$ and discarding the rest. This makes sense since the density of states $\rho(\omega)$ is the trace of the imaginary part of the Green function:

$$\rho(\omega) = -\frac{2}{N} \operatorname{Im} \sum_{\boldsymbol{r}} G_{\boldsymbol{r}\boldsymbol{r}}(\omega + i0^+) = -\frac{2}{N} \operatorname{Im} \sum_{\boldsymbol{k}} G(\boldsymbol{k}, \omega + i0^+) , \qquad (52)$$

and the spectral function $A(\mathbf{k}, \omega)$, as a partial trace, involves only the diagonal part. Moreover, because of the sum rule (12), which is basis independent, the frequency integral of the imaginary part of the off-diagonal components of the Green function vanishes.

Another possible formula for periodization is to apply relation (49) to the self-energy Σ instead. This is appealing since Σ is an irreducible quantity, as opposed to G, and amounts to throwing out the off-diagonal components of Σ before applying Dyson's equation to get G, as opposed to discarding the off-diagonal part at the last step, once the matrix inversion towards G has taken place. Unfortunately, this turns out not to work, which is not surprising given the nonlinear relation between Σ and the spectral function. As Fig. 3 shows, periodizing the Green function (Eq. (49)) reproduces the expected features of the spectral function of the one-dimensional Hubbard model: In particular, the Mott gap that opens at arbitrarily small U (as known from the exact solution). On the other hand, periodizing the self-energy leaves spectral weight within the Mott gap for an arbitrarily large value of U. This illustrates the correctness of Green function periodization.



Fig. 3: Left: CPT spectral function of the one-dimensional, half-filled Hubbard model with U = 4, t = 1, with Green function periodization (L = 16). Right: the same, with self-energy periodization instead; notice the important spectral weight in the middle of the Mott gap.



Fig. 4: Spectral function of the two-dimensional Hubbard model with band parameters t = 1, t' = -0.3 and t'' = 0.2. Top panel: different values of U for hole doping 1/6. Bottom panel: the same for electron doping 1/6. The pseudo-gap phenomenon manifests itself as the disappearance of the quasi-particle peak at the Fermi level along the side $(\pi, 0) - (\pi, \pi)$ in the hole-doped case, and along the diagonal $(0, 0) - (\pi, \pi)$ in the electron-doped case. Adapted from [4].

As an illustration of what can be revealed by the periodized CPT Green function, Fig. 4 shows the spectral function of the two-dimensional Hubbard model, with band parameters appropriate for cuprate superconductors: t'/t = -0.3 and t''/t = 0.2, where t' and t'' are second (diagonal) and third-neighbor hopping amplitudes, respectively. Several values of U were used, and two values of electron density: 5/6 (top) and 7/6 (bottom). We can see the emergence of the Hubbard bands and how the chemical potential ($\omega = 0$) is pinned to the lower and upper Hubbard bands, respectively. In the top panel, the quasi-particle weight at the Fermi surface disappears along the direction $(\pi, 0) - (\pi, \pi)$, whereas a well-defined quasi-particle peak remains along the diagonal direction $(0, 0) - (\pi, \pi)$. This is accentuated as U increases. In the electron-doped case, the roles of the two directions are reversed.

Averages of one-body operators In the (\mathbf{R}, \mathbf{k}) basis, Formula (26) for the ground state average of a one-body operator (23) becomes

$$\bar{\mathcal{O}} = \frac{1}{N} \sum_{\tilde{\boldsymbol{k}}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \left\{ \operatorname{tr} \left[\boldsymbol{s}(\tilde{\boldsymbol{k}}) \boldsymbol{G}(\tilde{\boldsymbol{k}}, i\omega) \right] - \frac{\operatorname{tr} \boldsymbol{s}(\tilde{\boldsymbol{k}})}{i\omega - p} \right\}$$
(53)

where all matrices are now of size M_{sc} and we assume that the matrix s is diagonal in k (translational invariance over the super-lattice).

The result (25) is quite general and could formally by expressed as $\overline{O} = \text{Tr}(s G)$ where the symbol Tr (with a capital 'T') stands for a functional trace, i.e., includes an integral over frequencies as well as a trace over site and band indices, including even the convergence correction (the last term of Eq. (53)). The above expression is basis-independent; in the full wave-vector basis of one-particle states, the frequency summand would take the following form:

$$\frac{1}{N} \sum_{\tilde{\boldsymbol{k}}, \tilde{\boldsymbol{k}}', \boldsymbol{K}, \boldsymbol{K}'} s(\tilde{\boldsymbol{k}} + \boldsymbol{K}, \tilde{\boldsymbol{k}}' + \boldsymbol{K}') G(\tilde{\boldsymbol{k}}' + \boldsymbol{K}', \tilde{\boldsymbol{k}} + \boldsymbol{K}, i\omega)$$
(54)

If the operator O is translationally invariant, as it usually is, then

$$s(\tilde{\boldsymbol{k}} + \boldsymbol{K}, \tilde{\boldsymbol{k}}' + \boldsymbol{K}') = \delta_{\boldsymbol{K}\boldsymbol{K}'} \,\delta_{\tilde{\boldsymbol{k}}\tilde{\boldsymbol{k}}'} \,s(\boldsymbol{k}) = \delta_{\boldsymbol{k}\boldsymbol{k}'} \,s(\boldsymbol{k}) \,, \tag{55}$$

and the above reduces to

$$\sum_{\boldsymbol{k}} s(\boldsymbol{k}) G_{\text{per.}}(\boldsymbol{k}, i\omega) , \qquad (56)$$

where $G_{\text{per.}}(\mathbf{k}, i\omega)$ is the periodized Green function (49). This means that expectation values of translationally invariant, one-body operators, computed in the periodization scheme (49), coincide with those computed without periodization, i.e., with Eq. (53). This does not hold for other periodization schemes (e.g. periodizing the self-energy), as it crucially depends on our discarding the off-diagonal elements of \mathbf{G} in the full wave-vector basis, which is possible because we take the trace of \mathbf{G} against a matrix \mathbf{s} that is itself diagonal in that basis.

3 The exact diagonalization method

This lecture is not about numerics. Nevertheless, it is important to understand some basic facts about the exact diagonalization technique for correlated systems at zero temperature in order to understand some of the constraints imposed on quantum cluster methods by computing resources.

Let us therefore consider a single cluster with M degrees of freedom labeled α, β , etc. and Hamiltonian H_c . The essential steps involved in computing the cluster Green function $G_{\alpha\beta}(z)$ in the exact diagonalization method are the following:

1. Coding the basis states. States in the Hilbert space are represented as $|\psi\rangle = \sum_i \psi_i |b_i\rangle$, where the $|b_i\rangle$ form a basis in which it must be convenient to compute the matrix elements of H_c , i.e., the matrix elements should not be too numerous. Because of the local two-body interaction term, the most convenient basis is local, i.e., is defined by occupation numbers of the Wannier orbitals:

$$|b(n_{\alpha})\rangle = (c_1^{\dagger})^{n_1} (c_2^{\dagger})^{n_2} \cdots (c_M^{\dagger})^{n_M} |0\rangle$$
 $n_{\alpha} = 0$ or 1 (57)

For M degrees of freedom (spin included), there are 2^M such states. However, various symmetries will make the Hamiltonian block-diagonal in this basis. The most obvious ones are particle number and spin conservation, if applicable. Then only a subset of dimension D of the 2^M basis states is needed. The actual states are then specified by a D-dimensional array ψ_i . If point group symmetries are taken into account, then things are slightly more complicated, but easily manageable if we only take care of Abelian symmetries. The important point is that the dimension of the Hilbert space grows exponentially with M and therefore only small clusters can be used. Even though a ground state computation can be performed on the Hubbard model with slightly over 20 sites if all symmetries are used in the normal state, such a size is not realistic for quantum cluster methods, in which the Green function must also be computed and where many sequential solutions are needed within self-consistent or variational procedures. At this time the sweet spot still lies around 12 sites (i.e. M = 24 with spin).

- 2. Building the Hamiltonian. The matrix elements of H_c must be computed. In principle they need not be stored in memory, i.e., they could be computed 'on the fly', as needed. However, if memory is less a problem than computing time, it is advantageous to store them and to build a sparse matrix for H_c , especially in a way that allows the matrix to be quickly updated when the parameters of H_c (the coefficients of the various terms) change, for instance between successive iterations of a self-consistent procedure.
- 3. Computing the ground state. Once a representation of the Hamiltonian H_c is at hand, the ground state $|\Omega\rangle$ is typically computed using the Lanczos method. The latter is an iterative procedure that starts from a random vector in the Hilbert space and, through successive applications of the matrix H_c , finds the lowest eigenvector of H_c with numerical

accuracy. For instance, if the dimension of the Hilbert space is $D \sim 10^6$, an accurate ground state is found with only a few hundred iterations. The procedure actually builds an orthonormal basis in the K-dimensional Krylov space based on a random initial vector $|\phi_0\rangle$:

$$\mathcal{K} = \operatorname{span}\left\{ |\phi_0\rangle, H_c |\phi_0\rangle, H_c^2 |\phi_0\rangle, \dots, H_c^{K-1} |\phi_0\rangle \right\}$$
(58)

In that basis, the Hamiltonian H_c is truncated into a simple tridiagonal form that is easily diagonalized. It can be shown that extreme eigenvectors are very well represented in \mathcal{K} .

4. Computing the Green function. Once the ground state |Ω⟩ is known, we need to apply definition (3) to compute the Green function. Once again, Krylov spaces are constructed. Two variants of the Lanczos method may be used, leading to two different data representations of the Green function. The first one proceeds by applying the usual Lanczos procedure, but on the states c_α |Ω⟩ and (c_α + c_β)|Ω⟩ (and their creation operator equivalent) instead of a random state. The Krylov spaces thus constructed provide a good representation of the action of the operator (z ± H)⁻¹ of Eq. (3). The second variant, called the *band Lanczos method*, constructs a generalized Krylov space generated from the set {c_α|Ω⟩} (or {c_α[†]|Ω⟩}) by successive application of H_c, and then uses the projection of H_c on that space to compute (3). It requires more memory than the first method but is faster. It also provides a spectral representation (11) of the Green function, albeit with a few hundred poles ω_r instead of a number of the order of the dimension of the Hilbert space, as in the exact result. Both representations of the cluster Green function allow it to be computed at any complex frequency z, provided we avoid the poles ω_r located on the real axis.

4 Cellular Dynamical Mean-Field Theory

Let us go back to the cluster decomposition (32) of the Hamiltonian. The main problem with CPT, i.e., with the prescription that $H_0^{(j)}$ is simply the restriction of H_0 to the cluster, is that the corresponding self-energy does not feel the effect of the lattice at all. It is the self-energy of a small system and thus cannot account for complex phenomena, such as phase transitions and spontaneously broken symmetry.

Therefore the main thrust of quantum cluster methods is to define $H_0^{(j)}$ in such a way as to represent as well as possible the effect of the lattice on the cluster. Perhaps the most elegant way to describe this is through the path integral formalism. The material of Sect. 4.1 is meant for readers familiar with that formalism. Others may skip straight to Sect. 4.2 if they wish.

4.1 The dynamical mean field

In the path integral formulation, the basic object is the partition function, whose expression is

$$Z = \int \prod_{\alpha} \left[\mathrm{d}c_{\alpha} \mathrm{d}\bar{c}_{\alpha} \right] \exp(iS[c,\bar{c}])$$
(59)

where the action S is

$$S[c,\bar{c}] = \int dt \left\{ \sum_{\alpha,\beta} \bar{c}_{\alpha}(t) \left(i\delta_{\alpha\beta}\partial_t - t_{\alpha\beta} \right) c_{\beta}(t) - H_1(c,\bar{c}) \right\}.$$
 (60)

The integral is carried out over a continuum of conjugate Grassmann variables $c_{\alpha}(t)$ and $\bar{c}_{\alpha}(t)$. An imaginary-time formulation is also possible and is necessary when dealing with finite temperatures; it is used to apply Monte Carlo sampling techniques.

In terms of the noninteracting Green function G_0 in the time domain, this may be written as

$$S[c,\bar{c}] = \int dt \, dt' \left\{ \sum_{\alpha,\beta} \bar{c}_{\alpha}(t) \, G_{0,\alpha\beta}^{-1}(t-t') \, c_{\beta}(t') - H_1(c,\bar{c}) \, \delta(t-t') \right\}.$$
 (61)

Following a tiling of the lattice with clusters, that action may be expressed as

$$S = \sum_{j} S^{(j)} + \sum_{i,j} S^{(i,j)} , \qquad (62)$$

where $S^{(j)}$ is the restriction of S to the cluster labeled j, and $S^{(i,j)}$ involve sites belonging to clusters i and j, typically inter-cluster hopping terms contained in the matrix $t^{(i,j)}$ of Eq. (29). CDMFT assumes that the effect of the environment of each cluster can be well approximated by an effective action

$$\sum_{i \in \Gamma} S^{(i,j)} \to S^{(j)}_{\text{env.}} .$$
(63)

Replacing the sum on the left by a single term for each cluster effectively decouples them. This contribution from the environment is assumed to be uncorrelated, i.e., to be quadratic in *c*. Thus, the total effective action for a given cluster takes the general form

$$S_{\text{eff}}[c,\bar{c}] = \int dt \, dt' \, \sum_{\alpha,\beta} \bar{c}_{\alpha}(t) \, \mathscr{G}_{0,\alpha\beta}^{-1}(t-t') \, c_{\beta}(t') + \int dt \, H_1(c,\bar{c}) \tag{64}$$

where \mathscr{G}_0 is the *dynamical mean field*. The indices α, β are now restricted to the same cluster, and likewise for the interaction Hamiltonian H_1 .

In the frequency domain the dynamical mean field can be written, in matrix form, as

$$\mathscr{G}_0^{-1}(\omega) = \omega - \boldsymbol{t}_c - \boldsymbol{\Gamma}(\omega), \qquad (65)$$

where t_c is the restriction of the hopping matrix to the cluster and $\Gamma(\omega)$, the hybridization function, represents the dynamical hybridization of the cluster orbitals with their effective environment. This is better expressed in terms of an Anderson impurity model [5]; let us explain. In order for this effective action to make sense, the dynamical mean field \mathscr{G}_0 must be causal. This implies that it must have the analytic properties of a Green function: The poles and zeros of its eigenvalues must lie on the real axis and the associated residues must be positive. In addition, $\mathscr{G}_0(\omega)$ must behave like $1/\omega$ at large frequencies. In other words, $\mathscr{G}_0(\omega)$ must have a spectral representation like Eq. (11). Consequently, the hybridization function must have a spectral representation (22) like that of a self-energy: 3

$$\Gamma_{\alpha\beta}(z) = \sum_{r}^{N_b} \frac{\theta_{\alpha r} \theta_{\beta r}^*}{z - \varepsilon_r}$$
(66)

as a function of a complex frequency z, where ε_r and $\theta_{\alpha r}$ form a collection of parameters that can be adjusted to fit any causal hybridization function as closely as needed. N_b is the number of poles deemed necessary to adequately represent the hybridization function.

4.2 The equivalent Anderson impurity model

Now, let us connect back with the Hamiltonian formalism. The effect of the cluster's environment, which is modeled by the hybridization function (66), may equivalently be represented by coupling the cluster with a set of N_b ancillary orbitals labeled by r, with annihilation operators a_r . The orbitals are uncorrelated, and form a *bath* in which the cluster is immersed, so to speak. The cluster dynamics is then described by the following Anderson impurity model:

$$H_{\text{AIM}} = \sum_{\alpha,\beta} t_{c,\alpha\beta} c^{\dagger}_{\alpha} c_{\beta} + \sum_{\alpha,r} \left(\theta_{\alpha r} c^{\dagger}_{\alpha} a_r + \text{H.c.} \right) + \sum_{r}^{N_{\theta}} \varepsilon_r a^{\dagger}_r a_r + H_1 .$$
(67)

Electrons can hop between the cluster sites labeled α, β and the bath orbitals.

Let us show how the hybridization function (66) emerges from this model. The Green function associated with the noninteracting Anderson model (if we drop H_1 from (67)) is simply

$$\boldsymbol{G}_{0}^{\mathrm{full}}(z) = \frac{1}{z - \boldsymbol{T}}$$
(68)

N,

where the full hopping matrix T for the combined cluster and bath system is

$$\boldsymbol{T} = \begin{pmatrix} \boldsymbol{t}_c & \boldsymbol{\theta} \\ \boldsymbol{\theta}^{\dagger} & \boldsymbol{\varepsilon} \end{pmatrix}.$$
 (69)

 t_c is the $M \times M$ hopping matrix within cluster degrees of freedom only, θ is the $M \times N_b$ hopping matrix between bath and cluster orbitals, and ε the diagonal $N_b \times N_b$ matrix of bath energies ε_{α} . The Green function obtained by tracing out the bath degrees of freedom is simply the restriction of G_{full} to the cluster degrees of freedom only. The mathematical problem at hand is simply to invert a 2 × 2 block matrix

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}^{-1}$$
(70)

where $A_{11} = z - t_c$, $A_{12} = A_{21}^{\dagger} = \theta$, $A_{22} = z - \varepsilon$, and B_{11} is the Green function we are looking for. By working out the inverse matrix condition, we find in particular that

$$A_{11}B_{11} + A_{12}B_{21} = \mathbf{1} B_{21} = -A_{22}^{-1}A_{21}B_{11} (71)$$

 $^{{}^{3}\}Gamma$ could also have a frequency-independent piece Γ^{∞} , but that piece turns out to be always zero in CDMFT, although this is not so in Potthoff's dynamical impurity approximation (DIA).



Fig. 5: *Example cluster-bath systems used in the ED implementation of CDMFT. (A) and (B):* 2-site, 4-bath systems used to study the one-dimensional Hubbard model. (C): a 4-site, 8-bath system used for the two-dimensional Hubbard model. See text for explanations.

and therefore

$$\left(A_{11} - A_{12}A_{22}^{-1}A_{21}\right)B_{11} = \mathbf{1}.$$
(72)

The noninteracting Green function of the cluster, G_{0c} , is thus given by

$$G_{0c}^{-1} = z - t_c - \Gamma(z)$$
 $\Gamma(z) = \theta \frac{1}{z - \varepsilon} \theta^{\dagger}$ (73)

where we recognize the hybridization function (66) in the last term. Note that the bath energy matrix ε can always be chosen to be diagonal, but does not have to be; Eq. (73) is valid even if ε is not diagonal.

In the interacting case, the only difference lies in the existence of the self-energy, which has no component in the bath since the latter is uncorrelated. We then have the relations

$$\boldsymbol{G}_{c}^{-1}(z) = z - \boldsymbol{t}_{c} - \boldsymbol{\Gamma}(z) - \boldsymbol{\Sigma}(z) = \boldsymbol{\mathscr{G}}_{0}^{-1}(z) - \boldsymbol{\Sigma}(z)$$
(74)

Solving the AIM on the cluster can be done in a variety of ways, for instance by exact diagonalization, but also by more traditional quantum Monte Carlo (QMC) approaches like the Hirsch-Fye method. Generally, the method used to compute $G_c^{-1}(z)$ is called the *impurity solver*, because of the AIM context, even though the problem does not involve physical impurities.

The continuous-time quantum Monte Carlo solver [6, 7] (CT-QMC) has been developed especially for the purpose of DMFT and CDMFT. It is an exact method, free of systematic errors, that works at finite temperature. It is however quite computationally intensive, and is also limited in practice to small clusters (but the bath is essentially infinite). All QMC methods are also affected by the fermion sign problem.

When using an exact diagonalization solver, the number of bath orbitals is very limited. Examples of cluster-bath systems are illustrated on Fig. 5. In system (A), each of the two cluster sites is hybridized with 2 bath orbitals exclusively. Left-right symmetry imposes the constraints

 $\varepsilon_3 = \varepsilon_1, \varepsilon_4 = \varepsilon_2, \theta_3 = \theta_1$ and $\theta_4 = \theta_2$. System (B) is more general: the bath orbitals are not hybridized with specific cluster sites, but with combinations of a given symmetry (here, even and odd orbitals $c_{\pm} = c_1 \pm c_2$). This approach, proposed in Ref. [8], is potentially more accurate, since the number of variational parameters is generally larger. System (C) is a 4-site cluster coupled to 8 bath orbitals. Again, symmetry considerations in the normal state will impose constraints on the values of the 16 parameters ε_i and θ_i . In principle, one may also introduce hopping terms between the bath orbitals (indicated by curved dashed lines); this would introduce additional bath parameters and therefore a richer representation of the hybridization function $\Gamma(z)$. In practice, anomalous hopping will be introduced along the curved dashed lines when studying superconductivity (see Sect. 5.2).

4.3 The self-consistency condition

How does one determine the hybridization function $\Gamma(z)$ so as to best represent the effect of the lattice environment on the cluster? Just like ordinary mean-field theory can be formulated equivalently either as a variational principle (Hartree-Fock theory) or via a self-consistency condition, so can dynamical mean-field theory. The variational approach is based on Potthoff's self-energy functional theory [9, 10] and is called the *dynamical impurity approximation* (DIA, or CDIA for its cluster extension). It has many advantages, both from the formal point of view and in practice, for some systems with small values of N_b solved by exact diagonalization, but we will not describe it here for lack of space. Interested readers can turn to Refs [11–13] for details. Historically and in most applications, the hybridization function is determined by applying a self-consistency principle that we will now describe.⁴

The approximate Green function of the lattice model that follows from the effective Hamiltonian (67) is constructed from the principle (28):

$$\boldsymbol{G}^{-1}(\boldsymbol{k}, z) = z - \boldsymbol{t}(\boldsymbol{k}) - \boldsymbol{\Sigma}(z) \quad , \tag{75}$$

where $t(\tilde{k})$ is the exact dispersion of the lattice model, expressed as a partial Fourier transform, i.e., as matrix in cluster indices with a dependence on the reduced wave-vector \tilde{k} defined in the Brillouin zone of the super-lattice.

Let us assume, for the time being, that the super-cell is made of a single cluster, so that Σ above is computed from the cluster Green function G_c (we will treat the case of multiple clusters later). Let us then Fourier transform $G(\tilde{k}, z)$ back to real-space, in order to project it onto the super-cell located at $\tilde{r} = 0$:

$$\bar{\boldsymbol{G}}(z) = \frac{L}{N} \sum_{\tilde{\boldsymbol{k}}} \left[z - \boldsymbol{t}(\tilde{\boldsymbol{k}}) - \boldsymbol{\Sigma}(z) \right]^{-1}$$
(76)

Ideally, this projected Green function \bar{G} should coincide with the cluster Green function G_c calculated from the dynamical mean field \mathscr{G}_0 . The condition $\bar{G} = G_c$ closes a self-consistency

⁴Contrary to mean-field theory, where the variational and self-consistent approaches yield the same solution, the self-consistent method followed in CDMFT does not yield the same solution as CDIA when the number of bath sites is finite.



Fig. 6: The CDMFT self-consistency loop.

loop, illustrated in Fig. 6, that hopefully converges towards an optimal dynamical mean field \mathscr{G}_0 . Let us summarize the elements of this loop:

- 1. An initial trial value of the dynamical mean field \mathscr{G}_0 is selected. With a QMC solver, this means choosing a Matsubara-frequency-dependent matrix $\Gamma(i\omega_n)$. With an ED solver applied to the Anderson impurity model (67), this means choosing an initial set of bath parameters $(\boldsymbol{\theta}, \boldsymbol{\varepsilon})$.
- 2. The impurity solver is applied, and G_c is computed, as well as the associated self-energy Σ , from Eq. (74).
- 3. The CPT Green function (75) is computed, as well as its projection \overline{G} onto the cluster.
- 4. The next step depends on whether one uses a QMC or an ED solver to compute G_c . In the QMC solver, one deals with the path integral formulation directly and the hybridization function $\Gamma(i\omega_n)$ is defined at Matsubara frequencies without reference to a bath of ancillary orbitals. Then the dynamical mean field is updated by substituting $G_c \to \overline{G}$ into Eq. (74):

$$\mathscr{G}_0^{-1}(i\omega_n) \leftarrow \bar{\mathbf{G}}^{-1}(i\omega_n) + \boldsymbol{\Sigma}(i\omega_n)$$
(77)

In the ED solver, the hybridization function is only known through Eq. (73) and the bath parameters θ and ε . Moreover, the number of adjustable bath parameters is finite, and therefore the self-consistency condition $\bar{G} = G_c$ cannot be satisfied exactly for all frequencies; it can only be optimized. This is done by minimizing the following "distance

function"

$$d(\boldsymbol{\theta}, \boldsymbol{\varepsilon}) = \sum_{i\omega_n} W(i\omega_n) \operatorname{tr} \left| \boldsymbol{G}_c^{-1}(i\omega_n) - \bar{\boldsymbol{G}}^{-1}(i\omega_n) \right|^2$$
(78)

where the sum is carried over a finite set of Matsubara frequencies associated with a fictitious temperature T, with weights $W(i\omega_n)$ used to emphasize low frequencies. This minimization is done numerically by any classic optimization method, simply by applying Eq. (73), without recomputing Σ ; it usually does not contribute appreciably to the total computing time. The outcome is a new set of bath parameters (θ, ε) , and therefore a new hybridization function.

5. One goes back to step 2, until \mathscr{G}_0 (or $\boldsymbol{\Gamma}$) converges.

4.4 Inhomogeneous systems

Let us now consider a super-cell made of n > 1 clusters. This may be needed if a single cluster does not tile the lattice, but two are necessary, like in Fig. 1. It is also needed for inhomogeneous systems where translational invariance is lost, at least on a length scale that involves many clusters. The notation of Eqs. (28) and (29) may still be used, except that n is no longer the total number of clusters on the lattice, but the number of clusters in the super-cell, so that each of the blocks $t^{(i,j)}$ will depend on the reduced wave-vector \tilde{k} . The inverse CPT Green function therefore has the form

$$\mathbf{G}^{-1}(\tilde{\mathbf{k}}, z) = z - \mathbf{t}(\tilde{\mathbf{k}}) - \mathbf{\Sigma}(z)
= \begin{pmatrix} z - \mathbf{t}^{(11)}(\tilde{\mathbf{k}}) - \mathbf{\Sigma}_{1}(z) & -\mathbf{t}^{(12)}(\tilde{\mathbf{k}}) & \dots & -\mathbf{t}^{(1n)}(\tilde{\mathbf{k}}) \\ -\mathbf{t}^{(21)}(\tilde{\mathbf{k}}) & z - \mathbf{t}^{(22)}(\tilde{\mathbf{k}}) - \mathbf{\Sigma}_{2}(z) & \dots & -\mathbf{t}^{(2n)}(\tilde{\mathbf{k}}) \\ \vdots & \vdots & \ddots & \vdots \\ -\mathbf{t}^{(n1)}(\tilde{\mathbf{k}}) & -\mathbf{t}^{(n2)}(\tilde{\mathbf{k}}) & \dots & z - \mathbf{t}^{(nn)}(\tilde{\mathbf{k}}) - \mathbf{\Sigma}_{n}(z) \end{pmatrix}$$
(79)

Some of the clusters may be connected only to other clusters of the same super-cell, not to clusters of the neighboring super-cells; therefore for those clusters, the matrix $t^{(ij)}$ is constant, i.e., does not depend on \tilde{k} .

As before, we define the projected local Green function (76), but this time \bar{G} has a block-matrix structure like that of Eq. (79). Let $\bar{G}^{(j)}$ denote the j^{th} diagonal block of \bar{G} . The self-consistency condition is modified so as to match $\bar{G}^{(j)}$ to the cluster Green function $G^{(j)}$ computed from the impurity solver. In particular, in the ED framework, the distance function (78) has the form

$$d(\boldsymbol{\theta}, \boldsymbol{\varepsilon}) = \sum_{i\omega_n, j} W(i\omega_n) \operatorname{tr} \left| \boldsymbol{G}^{(j)-1}(i\omega_n) - \bar{\boldsymbol{G}}^{(j)-1}(i\omega_n) \right|^2.$$
(80)

The bath parameters of all clusters in the super-cell contribute to any $\bar{G}^{(j)}$, and thus all clusters are coupled. The distance function is a sum over *n* separate terms (one for each cluster), each with its own set of bath parameters and hybridization function $\Gamma^{(j)}(z)$. Thus minimizing each of these terms separately will minimize their sum and vice versa.



Fig. 7: Super-cell of 19 six-site clusters used in Ref. [14] in order to study the effect of a repeated non-magnetic impurity (located at the central site) on the Hubbard model defined on the graphene lattice. The local magnetization is indicated by filled red (up) and open blue (down) circles respectively (the area of each circle is proportional to $\langle S_r^z \rangle$).

This approach was called I-CDMFT in Ref. [14]. In that work, it was applied to the problem of a repeated, non-magnetic impurity in graphene. From previous mean-field calculations, it was known that antiferromagnetic correlations arising from the impurity go well beyond nearest neighbors [15, 16]. In order to isolate the magnetism resulting from a single impurity, and at the same time avoid edge effects, the impurity was repeated periodically, i.e., a super-cell of 19 six-site clusters was defined (see Fig. 7). The impurity, characterized by a local energy $H_{\text{imp.}} = h n_0$, where 0 labels the impurity site, is located on the middle cluster. Fig. 7 shows the local magnetization induced by such an impurity on the Hubbard model defined on the graphene lattice, with parameters U = 2 and h = 11 (the nearest-neighbor hopping amplitude t is set to unity).

5 Applications

5.1 The Mott transition

A key success of Dynamical Mean-Field Theory is the picture it provides of the Mott metalinsulator transition. Consider Fig. 8, which shows the qualitative phase diagram in the U-Tplane of the half-filled, particle-hole symmetric Hubbard model. The left panel shows the prediction of single-site DMFT [17]. The Mott transition in the U-T plane is of first order, indicated as a red line on the figure. This first-order line ends at a finite-temperature critical point and at $U_{c1(0)}$, with a region (colored area) where the metallic and insulating phases may coexist. This single-site DMFT picture of the Mott transition has been criticized, mainly on



Fig. 8: Schematic phase diagram of the half-filled, particle-hole symmetric Hubbard model using single-site DMFT (left), CDMFT with a CT-QMC solver on a 2×2 plaquette (center) and the Dynamical Impurity Approximation (right). The red dots are the end of the first-order lines and therefore critical points. Adapted from [19].

the ground that the absence of feedback of magnetic correlations on single particle excitations yields a nonzero ground-state entropy ($S = N \ln 2$, N being the number of sites) in the Mott phase, and that this exaggerates the stability of the insulating phase at nonzero temperature. Cluster Dynamical Mean Field Theory modifies this picture by the addition of short-range correlation effects or, said otherwise, by adding a momentum-dependence to the self-energy. This provides a feedback of short-range antiferromagnetic fluctuations into single-particle properties. However, the main features of the DMFT picture are not affected by these refinements. The middle diagram of Fig. 8 emerges from a CDMFT study using the continuous-time QMC solver [18]. The essential difference with the single-site result is that the first-order line ends at $U_{c2}(0)$ instead of $U_{c1}(0)$ at zero temperature. The zero-temperature points are the result of an extrapolation, since QMC solvers were used in both cases. The right panel of Fig 8 is a modified scenario inspired by the Dynamical Impurity Approximation (DIA) [19], in which only the zero-temperature axis was actually calculated, with an exact diagonalization solver. It was shown in Ref. [19] that the transition is of first order even at zero temperature; the transition (red line) occurs when the ground state energies of the metallic and insulating solutions cross. As a function of U, a hysteresis loop was observed for the various bath parameters.

Regarding Fig. 8, we note that the slope of the first-order line is negative in the single-site DMFT solution, but positive in the CDMFT solution. Through the Clausius-Clapeyron equation, this implies that the entropy is larger in the Mott phase than in the metallic phase according to the single-site solution, whereas the opposite is true according to the CDMFT solution. This is another sign that the degeneracy of a single site exaggerates the entropy of the insulating state in DMFT.

Figure 9 shows the evolution of the local density of states $A(\omega)$ (DoS) across the Mott transition. The DoS on the left half of each panel (U = 5.0 and U = 5.6) are computed in the metallic solution, and those on the right (U = 5.4 and U = 5.8) in the insulating solution. The middle points (U = 5.4 and U = 5.6) are in the coexistence region. The bath used in the CT-QMC solution is effectively infinite, whereas the bath used with the ED solver has only 8 orbitals and is based on the system illustrated in Fig. 5C. Accordingly, the spectral function contains



Fig. 9: Evolution of the local density of states $A(\omega)$ across the Mott transition, for the squarelattice Hubbard model. Left panel: CT-QMC solver, from Ref. [18]. Right panel, ED solver, but with the CDIA, based on solutions found in Ref. [19].

traces of the discreteness of the bath, even though a Lorentzian broadening of the poles was used. Nevertheless, the same physics occurs at the same value of U/t in the two methods. The self-consistency condition $\bar{G} = G'$, in the bath parametrization used in [19], does not show a first-order transition (and a coexistence region) in that case; the latter can only be seen by solving the more exact conditions defined in the CDIA.

5.2 Superconductivity

Many of the theoretical approaches described in this volume were motivated by the ambition to explain the origin of high-temperature superconductivity, more specifically to answer the following question: does the Hubbard model contain the key elements to explain superconductivity in the cuprates? Single-site DMFT alone cannot answer this question, as it lacks the short-range correlation effects needed to even describe *d*-wave superconductivity. But the question has been addressed by quantum cluster methods: DCA, VCA, and CDMFT.

First of all, let us explain how superconductivity may be incorporated in the Green function formalism. The standard theoretical description of superconductivity involves a spontaneous violation of charge conservation, which translates into a nonzero expectation value of the operator $\hat{\Psi}$ that creates a uniform distribution of Cooper pairs. In a one-band model, this is

$$\hat{\Psi} = \frac{1}{N} \sum_{\boldsymbol{r}, \boldsymbol{r}'} g_{\boldsymbol{r}\boldsymbol{r}'} \left[c_{\boldsymbol{r}\uparrow} c_{\boldsymbol{r}\downarrow} - c_{\boldsymbol{r}\downarrow} c_{\boldsymbol{r}\uparrow\uparrow} \right].$$
(81)

In momentum space, this becomes

$$\hat{\Psi} = \frac{1}{N} \sum_{\boldsymbol{k}} g(\boldsymbol{k}) \left[c_{\uparrow}(\boldsymbol{k}) c_{\downarrow}(-\boldsymbol{k}) - c_{\downarrow}(\boldsymbol{k}) c_{\uparrow}(-\boldsymbol{k}) \right], \qquad (82)$$

with the correspondence

$$g(\boldsymbol{k}) = \sum_{\boldsymbol{r}} g_{\boldsymbol{r},0} \ e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} , \qquad (83)$$

where the pairing amplitude $g_{rr'}$ is assumed to depend only on r - r'. This amplitude is, roughly speaking, the Cooper pair's wave-function as a function of the relative position of the two electrons.

A nonzero value of $\langle \hat{\Psi} \rangle$ can only be established if the anomalous Green function (the *Gorkov function*) is nonzero:

$$F_{\boldsymbol{r}\boldsymbol{r}'}(z) = \langle \Omega | c_{\boldsymbol{r}\uparrow} \frac{1}{z - H + E_0} c_{\boldsymbol{r}\downarrow} | \Omega \rangle + \langle \Omega | c_{\boldsymbol{r}\downarrow\downarrow} \frac{1}{z + H - E_0} c_{\boldsymbol{r}\uparrow} | \Omega \rangle$$
(84)

The order parameter ψ is then the frequency integral of the Gorkov function, just like ordinary operators in Eq. (53):

$$\psi = \langle \hat{\Psi} \rangle = \frac{1}{N} \sum_{\tilde{k}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \left[g_{RR'}(\tilde{k}) F_{R'R}(\tilde{k}, i\omega) \right]$$
(85)

(we have used the (\mathbf{R}, \mathbf{k}) basis in the above formula). In order to smoothly integrate the Gorkov function into the formalism we have developed so far, the Nambu formalism is used: we perform a particle-hole transformation on the spin down sector and work with the operators $d_{r\sigma} = (c_{r\uparrow}, c_{r\downarrow}^{\dagger})$. These still obey the anticommutation relations $\{d_{r\sigma}, d_{r'\sigma'}^{\dagger}\} = \delta_{rr'}\delta_{\sigma\sigma'}$. In terms of these operators, the pairing operator $\hat{\Psi}$ takes the form of a hopping term because only destruction operators of opposite spins are multiplied. Thus, if we apply to the $d_{r\sigma}$ and $d_{r\sigma}^{\dagger}$ the definition (3) of the Green function and write it in block form to reveal the spin components, we find

$$\boldsymbol{G}(z) = \begin{pmatrix} \boldsymbol{G}_{\uparrow}(z) & \boldsymbol{F}(z) \\ \boldsymbol{F}^{\dagger}(z) & -\boldsymbol{G}_{\downarrow}(z) \end{pmatrix}$$
(86)

where G_{\uparrow} and G_{\downarrow} only involve up and down spins, respectively. As long as there are no spinflip terms in the Hamiltonian, the Gorkov function can be included in this way in the Green function (spin-flip terms would spoil the process, as they would look like anomalous terms after the particle-hole transformation).

In order to probe for superconductivity in CDMFT, the hybridization function (73) must contain anomalous terms. Within the ED solver, this was at first accomplished as illustrated on Fig. 5C, i.e., by adding to the bath Hamiltonian *d*-wave pairing terms between bath orbitals themselves (the red dotted lines of Fig. 5C). In this parametrization, the bath is seemingly made of two "ghost clusters" whose pairing terms mimic the broken symmetry state that could take place on the cluster itself. Note that CDMFT does not tamper with the cluster Hamiltonian when probing broken symmetries. The agents of symmetry breaking are rather concentrated in the bath.

Any study of *d*-wave superconductivity within the square-lattice Hubbard model must also take into account the possibility of antiferromagnetic order in competition, or in coexistence with, superconductivity. This requires a more general bath parametrization, with different bath energies and hybridization for the two magnetic sub-lattices and spin projections. The reduced symmetry would translate into the following constraints on the parameters defined in Fig. 5C:

$$\varepsilon_{1\sigma} = \varepsilon_{4\sigma} = \varepsilon_{2-\sigma} = \varepsilon_{3-\sigma} \quad \text{and} \quad \varepsilon_{5\sigma} = \varepsilon_{8\sigma} = \varepsilon_{6-\sigma} = \varepsilon_{7-\sigma}$$
(87)



Fig. 10: Left panel top: d-wave order parameter ψ as a function of electron density n, for various values of U and t' = -0.3t, t'' = 0.2t. Bottom: the same, scaled by $J = 4t^2/U$. Right panel: d-wave (ψ) and antiferromagnetic (M) order parameters vs. n, from a common solution where they are allowed to compete. Taken from Ref. [20].

and likewise for θ_i . The independent bath parameters would then be $\varepsilon_{1,\uparrow}$, $\varepsilon_{1,\downarrow}$, $\varepsilon_{2,\uparrow}$, $\varepsilon_{2,\downarrow}$, the corresponding values of θ_i , and two in-bath pairing operators.

Figure 10, taken from Ref. [20], shows the result of a CDMFT computation on the one-band Hubbard model with a tight binding dispersion appropriate for a cuprate superconductor like YBCO, with diagonal hopping t' = -0.3t and third-neighbor hopping t'' = 0.2t. Both the *d*-wave order parameter ψ and the antiferromagnetic order parameter M are shown, where

$$M = \langle \hat{M} \rangle \qquad \qquad \hat{M} = \frac{1}{N} \sum_{\boldsymbol{r}} e^{i \boldsymbol{Q} \cdot \boldsymbol{r}} \left(n_{\boldsymbol{r}\uparrow} - n_{\boldsymbol{r}\downarrow} \right) \qquad \boldsymbol{Q} = (\pi, \pi) \quad . \tag{88}$$

There is a region of doping where the two phases compete and coexist at a microscopic scale (right panel of Fig. 10). One sees (left panel of Fig. 10) that the superconducting order parameter scales like $J = 4t^2/U$, at least in the under-doped region.

The CT-QMC solver was applied to the superconductivity problem in Ref. [21], in the special case t' = 0. The CT-QMC allows for an estimate of T_c , but such a computation is very resourceintensive because of critical slowing down. Of course, this T_c has a mean-field character: The Mermin-Wagner theorem forbids the spontaneous breakdown of continuous symmetries in a purely two-dimensional system at nonzero temperature. In a finite cluster, the long wavelength pair fluctuations that would destabilize a superconducting phase at finite temperature are not at work and cannot be accounted for by a fermionic bath.

A fair criticism of the above results on broken symmetries in the Hubbard model is the lack of finite-size analysis. The existence of broken symmetry phases, such as antiferromagnetism and *d*-wave superconductivity, can only be established firmly in the limit of infinite cluster size; an infinite bath-size is not sufficient. In principle infinite-size extrapolations should be performed in order to assess the robustness of CDMFT predictions in the thermodynamic limit. In practice, this requires vast amounts of computing resources and a solver that can accommodate larger clusters, such as the Hirsch-Fye QMC or the auxiliary-field CT-QMC [22]. This was accomplished within the dynamical cluster approximation (DCA) in Ref. [23], with cluster sizes ranging up to L = 32 and special attention paid to the cluster shape in relation to the periodic boundary conditions used in DCA. The existence of a Kosterlitz-Thouless transition was confirmed in the square-lattice Hubbard model at $T_c \approx 0.023t$ for U = 4t and $\delta \approx 10\%$. The cost of these computations precluded a wider exploration of parameter space. The assumption underlying current work on superconductivity using cluster approaches is that the thermodynamic limit will bring important renormalizations but will not qualitatively affect the dependence of the superconducting order upon band parameters, interaction strength, or doping. Thus, cluster approaches are important tools in exploring the space of models that can potentially lead to superconductivity or other broken symmetry phases.

6 Extended interactions

The cluster methods discussed above only apply to systems with on-site interactions, such as the simple Hubbard model (1), as the interaction $H_1^{(j)}$ on each cluster was supposed to be the restriction to the cluster of the full interaction H_1 . This is no longer true in the *extended* Hubbard model, in which the Coulomb interaction between electrons residing on different Wannier orbitals is included:

$$H_{V} = \frac{1}{2} \sum_{\boldsymbol{r}, \boldsymbol{r}'} V_{\boldsymbol{r}'\boldsymbol{r}} \, n_{\boldsymbol{r}'} n_{\boldsymbol{r}}$$
(89)

(the factor 1/2 is there to avoid double counting the pairs (r, r')). Treating such a model with quantum cluster approaches requires an additional approximation: One applies the Hartree approximation on the extended interactions that straddle different clusters but treats exactly all interactions within each cluster. This is called the dynamical Hartree approximation (DHA). It has been used in Ref. [24, 25] in order to assess the effect of such interactions on stronglycorrelated superconductivity.

In the DHA, the extended interaction (89) is separated into two terms:

$$\frac{1}{2} \sum_{\boldsymbol{r}, \boldsymbol{r}'} V_{\boldsymbol{r}, \boldsymbol{r}'}^{c} n_{\boldsymbol{r}} n_{\boldsymbol{r}'} + \frac{1}{2} \sum_{\boldsymbol{r}, \boldsymbol{r}'} V_{\boldsymbol{r}, \boldsymbol{r}'}^{ic} n_{\boldsymbol{r}} n_{\boldsymbol{r}'}$$
(90)

where $V_{\mathbf{r},\mathbf{r}'}^{c}$ denotes the extended interaction between sites belonging to the same cluster and $V_{\mathbf{r},\mathbf{r}'}^{ic}$ those interactions between sites belonging to different clusters. Each number operator appearing in the second term is then written as $n_{\mathbf{r}} = \bar{n}_{\mathbf{r}} + \delta n_{\mathbf{r}}$, where $\bar{n}_{\mathbf{r}} = \langle n_{\mathbf{r}} \rangle$ is the average value of $n_{\mathbf{r}}$ and $\delta n_{\mathbf{r}}$, by definition, its fluctuation. The classic mean-field treatment is then applied:

$$n_{\boldsymbol{r}}n_{\boldsymbol{r}'} = \bar{n}_{\boldsymbol{r}}\bar{n}_{\boldsymbol{r}'} + \delta n_{\boldsymbol{r}}\bar{n}_{\boldsymbol{r}'} + \bar{n}_{\boldsymbol{r}}\delta n_{\boldsymbol{r}'} + \delta n_{\boldsymbol{r}}\delta n_{\boldsymbol{r}'}$$
(91)

and the last term is dropped, as fluctuations are deemed small. Substituting $\delta n_r = n_r - \bar{n}_r$ in



Fig. 11: *Phase diagram of the half-filled extended Hubbard model defined on the graphene lattice. U and V are the on-site and nearest-neighbor repulsion, respectively. See text for details. Adapted from Refs* [25] *and* [26].

the rest, we end up with the replacement

$$\frac{1}{2} \sum_{\boldsymbol{r},\boldsymbol{r}'} V_{\boldsymbol{r},\boldsymbol{r}'}^{\rm ic} \, n_{\boldsymbol{r}} n_{\boldsymbol{r}'} \to \hat{V}^{\rm ic} = \frac{1}{2} \sum_{\boldsymbol{r},\boldsymbol{r}'} V_{\boldsymbol{r},\boldsymbol{r}'}^{\rm ic} \left(\bar{n}_{\boldsymbol{r}} n_{\boldsymbol{r}'} + n_{\boldsymbol{r}} \bar{n}_{\boldsymbol{r}'} - \bar{n}_{\boldsymbol{r}} \bar{n}_{\boldsymbol{r}'} \right). \tag{92}$$

These are local, one-body terms only and therefore are included in the non-interacting piece H_0 . Because of translation symmetry on the super-lattice, the averages \bar{n}_r must be the same in each super-cell, and therefore the above term can be determined within a super-cell only, and the matrix $V_{r,r'}^{ic}$ can be viewed as acting on the sites of the super-cell only. Of course, interactions straddling different super-cells are "folded back" into a single super-cell.

The averages \bar{n}_r must be determined self-consistently. In a CPT computation, this calls for a self-consistent procedure whereby \bar{n}_r is computed at each step with the help of Eq. (53) and its value injected in a new H_0 , etc. In CDMFT, computing the averages can be done within the existing self-consistency loop of Fig. 6, e.g., at the same step where \bar{G} is computed. Thus, the mean fields \bar{n}_r are converged at the same time as the hybridization function Γ and the DHA adds very little overhead to the existing CDMFT procedure, although it is conceivable that more iterations are needed for convergence.

Instead of treating each operator n_r separately in the DHA, it is often advantageous to diagonalize the symmetric matrix $V_{r,r'}^{ic}$ and to express the mean field problem in terms of eigenoperators m_k , which are linear combinations of the different n_r 's of the cluster:

$$\hat{V}^{\rm ic} = \sum_{k} V_k^{\rm ic} \left[\bar{m}_k m_k - \frac{1}{2} \bar{m}_k^2 \right] \tag{93}$$

where V_k^{ic} is an eigenvalue of the matrix $V_{r,r'}^{ic}$ defined in the super-cell. The use of eigenoperators allows one to select or suppress different channels for charge-density-wave instabilities. For instance, Fig. 11 shows the phase diagram of the extended Hubbard model on the graphene lattice. Only on-site (U) and nearest-neighbor (V) interactions were considered. If V is large enough, a charge-density-wave sets in with different densities on the A and B sub-lattices. The DHA was used to find the phase boundary between the homogeneous solution (N) and the charge density wave (CDW), by including selectively the eigenoperator m_k associated with the CDW and by comparing the energy of the two solutions. The transition between the two phases becomes discontinuous (first-order) at some value of U. The results of the DHA are compared with those of DCA computations performed on larger clusters in Ref. [26]. The strong coupling limit of the phase boundary is known to be the straight line U = 3V (dashed line on the figure).

Concluding remarks

Quantum cluster methods provide a unique window into the physics of strongly correlated materials. They capture short-distance correlations exactly in models of strongly correlated electrons and thus can describe phenomena that are not accessible to mean-field-like approaches. For instance, the effective, dynamic attraction between electrons located on nearest-neighbor sites in the Hubbard model, which leads to pairing and superconductivity in that model, is captured by CDMFT on a 4-site cluster. These methods are so far limited to rather small clusters or by other issues affecting various impurity solvers, like the sign problem in QMC, etc. But they constitute a framework that motivates continuous improvement in impurity solvers and that opens up lines of inquiry that were previously limited.

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