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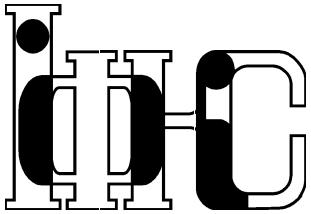

**ІНСТИТУТ ФІЗИКИ КОНДЕНСОВАНИХ СИСТЕМ**

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# NONEQUILIBRIUM DYNAMICAL MEAN-FIELD THEORY FOR THE CHARGE-DENSITY-WAVE PHASE OF THE FALICOV-KIMBALL MODEL

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**Анотація.** Розвинено нерівноважну теорію динамічного середнього поля для опису впорядкованої низькотемпературної фази з періодичною модуляцією густини заряду. Розглядається безспінова модель Фалікова-Кімбала, яка може бути розв'язана точно. До такої сильноскорельованої системи прикладається просторово однорідне постійне електричне поле. Представлено послідовне виведення функцій Ґріна, які означені на часовому контурі Келдиша-Швінґера, в нерівноважній теорії динамічного середнього поля. Також, обговорюються методи розв'язання системи пов'язаних рівнянь.

**Nonequilibrium dynamical mean-field theory for the charge-density-wave phase of the Falicov-Kimball model**

O.P. Matveev, J.K. Freericks, A.M. Shvaika

**Abstract.** Nonequilibrium dynamical mean-field theory is developed for the case of a low-temperature ordered phase with a periodic modulation of the charge density. We consider the spinless Falicov-Kimball model which can be solved exactly. This strongly correlated system is then placed in an uniform external dc electric field. We present a complete derivation for nonequilibrium dynamical mean-field theory Green's functions defined on the Keldysh-Schwinger time contour. We also discuss techniques used to solve the coupled equations.





## 1. Introduction

There are a number of strongly correlated materials that have charge-density-wave (CDW) behavior. Static order occurs in the transition metal di- and trichalchogenides, which display either quasi one dimensional ($NbSe_3$) or quasi two dimensional ($TaSe_2$ or $TbTe_3$) structures [1–3]. Three-dimensional charge-density-wave order is observed in $BaBiO_3$ and $Ba_{1-x}K_xBiO_3$ compounds [4]. There is a longstanding question concerning the nature of the CDW order, namely, whether the order is driven electronically, with a lattice instability following the electronic instability, or *vice versa*. Indeed, in real materials the charge and lattice degrees of freedom are usually strongly coupled, but recent time-resolved core-level photoemission spectroscopy experiments [5] for CDW materials indicate an electronically driven nature to ordering. This makes it reasonable to study the CDW phase for the strongly correlated electronic systems that do not include a coupling to the lattice.

While most theoretical interests in strongly correlated systems have been concentrated on equilibrium behavior, recent experiments on pump-probe spectroscopy [5–10] has caused an increase of attention to nonequilibrium dynamics. These experiments display a nonequilibrium melting of the CDW state, which is manifested by a filling of the gap in the photoemission spectrum, while the order parameter remains nonzero. This phenomenon has been examined with an exactly solvable model [11, 12] for an initial system starting at zero temperature; nonzero temperatures have not been investigated yet.

We use the Falicov-Kimball model in our analysis because it is one of the simplest models [13] which possesses static charge-density-wave ordering and has an exact solution within equilibrium dynamical mean-field theory [14] (DMFT) (for a review see Ref. [15]). The many-body formalism for nonequilibrium dynamical mean-field theory is straightforward to develop within the Kadanoff-Baym-Keldysh formalism [16, 17]. Since the many-body perturbation theory diagrams are topologically identical for both equilibrium and nonequilibrium perturbation theories [18], the perturbative analysis of Metzner [19] guarantees that the nonequilibrium self-energy is also local in DMFT. Hence, the nonequilibrium DMFT lattice problem can be mapped onto an impurity one in a time-dependent field, just like the equilibrium problem, except now the fields have two-time arguments. The basic structure of the iterative approach to solving the DMFT equations [20] continues to hold. Detailed development of the nonequilibrium DMFT approach has been done for the case of the uniform phase of the Falicov-Kimball model [21–23]. Here

we generalize this method to the case of the charge-density-wave ordered phase.

## 2. Static order and the Hamiltonian

In order to describe the CDW ordered state, one has to rewrite the Hamiltonian assuming the existence of the charge modulation. This can be done in two ways: by introducing two sublattices "$A$" and "$B$" in real space or by the nesting of the Brillouin zone (BZ) at the modulation vector $\mathbf{Q} = (\pi, \pi, \dots)$ in a reciprocal space. The modulation vector $\mathbf{Q}$ defines the sublattices by

$$e^{i\mathbf{Q}\mathbf{R}_i} = \begin{cases} 1, & \mathbf{R}_i \in A, \\ -1, & \mathbf{R}_i \in B. \end{cases} \tag{2.1}$$

In the ordered phase, due to nesting of the Fermi surface, the BZ is reduced and instead of the annihilation (creation) operators with momentum $\mathbf{k}$ defined in the initial BZ by

$$c_{\mathbf{k}} = \frac{1}{N}\sum_i e^{i\mathbf{k}\mathbf{R}_i} c_i \tag{2.2}$$

one has to introduce two fermionic operators in momentum space in the reduced zone ($\mathbf{k} \in$ rBZ):

$$\tilde{c}_{1\mathbf{k}} = c_{\mathbf{k}} \qquad \text{and} \qquad \tilde{c}_{2\mathbf{k}} = c_{\mathbf{k}+\mathbf{Q}}. \tag{2.3}$$

Now, starting from Eq. (2.2) one can write down the relations between annihilation (creation) operators defined on the sublattices $(A, B)$ and in the reduced BZ $(1, 2)$

$$\begin{aligned} \tilde{c}_{1\mathbf{k}} &= \frac{1}{N}\sum_{i\in A} e^{i\mathbf{k}\mathbf{R}_i} c_i + \frac{1}{N}\sum_{i\in B} e^{i\mathbf{k}\mathbf{R}_i} c_i = \frac{1}{\sqrt{2}}(c_{\mathbf{k}A} + c_{\mathbf{k}B}), \\ \tilde{c}_{2\mathbf{k}} &= \frac{1}{N}\sum_{i\in A} e^{i(\mathbf{k}+\mathbf{Q})\mathbf{R}_i} c_i + \frac{1}{N}\sum_{i\in B} e^{i(\mathbf{k}+\mathbf{Q})\mathbf{R}_i} c_i = \frac{1}{\sqrt{2}}(c_{\mathbf{k}A} - c_{\mathbf{k}B}). \end{aligned} \tag{2.4}$$

This unitary transformation can be rewritten in a matrix form as follows:

$$\begin{bmatrix} \tilde{c}_{1\mathbf{k}} \\ \tilde{c}_{2\mathbf{k}} \end{bmatrix} = \hat{U} \begin{bmatrix} c_{\mathbf{k}A} \\ c_{\mathbf{k}B} \end{bmatrix}, \quad \text{where} \quad \hat{U} = \begin{Vmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{Vmatrix}. \tag{2.5}$$



The annihilation and creation operators connected by such transformations satisfy the commutation relations

$$[\tilde{c}_{m\mathbf{k}}, \tilde{c}^{\dagger}_{n\mathbf{k}'}]_+ = \delta_{\mathbf{k},\mathbf{k}'}\delta_{m,n}, \qquad m, n = 1, 2 \tag{2.6}$$

and

$$[c_{\mathbf{k},\alpha}, c^{\dagger}_{\mathbf{k}',\beta}]_+ = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\alpha,\beta}, \qquad \alpha, \beta = A, B. \tag{2.7}$$

We use both sublattice $(A, B)$ and reduced BZ $(1, 2)$ bases in our further derivations. Any two-operator-product-type quantity, e.g. the one-particle Green's function, can be defined with the additional sublattice indices

$$\hat{\mathcal{O}}(\mathbf{k}) = \|\mathcal{O}_{\alpha,\beta}(\mathbf{k})\|, \quad \alpha, \beta = A, B,$$

or with the reduced BZ indices

$$\hat{\tilde{\mathcal{O}}}(\mathbf{k}) = \|\mathcal{O}_{m,n}(\mathbf{k})\|, \quad m, n = 1, 2,$$

and these representations are connected by the aforementioned unitary transformation

$$\hat{\tilde{\mathcal{O}}}(\mathbf{k}) = \hat{U}\hat{\mathcal{O}}(\mathbf{k})\hat{U}^{-1}. \tag{2.8}$$

Next, we introduce the time-dependent Hamiltonian of our system. We consider the case, when charged fermions interact with an external uniform electric field. We assume that the field is spatially uniform and ignore all magnetic field and relativistic effects. This allows us to describe the electric field via a time-dependent vector potential in the Coulomb gauge as follows:

$$\mathbf{E}(t) = -\frac{1}{c}\frac{d}{dt}\mathbf{A}(t). \tag{2.9}$$

The time-dependent Hamiltonian of the spinless Falicov-Kimball model on a bipartite lattice ($\alpha, \beta = A, B$) has the form

$$\mathcal{H}(t) = \sum_{i\alpha} \mathcal{H}_i^{\alpha} - \sum_{ij\alpha\beta} t_{ij}^{\alpha\beta}(t) c^{\dagger}_{i\alpha} c_{j\beta}, \tag{2.10}$$

where the local term is equal to

$$\mathcal{H}_i^{\alpha} = U n_{id}^{\alpha} n_{if}^{\alpha} - \mu_d^{\alpha} n_{id}^{\alpha} - \mu_f^{\alpha} n_{if}^{\alpha}, \tag{2.11}$$

with the number operators of the itinerant and localized electrons given by $\hat{n}_{id}^{\alpha} = \hat{c}^{\dagger}_{i\alpha}\hat{c}_{i\alpha}$ and $\hat{n}_{if}^{\alpha} = \hat{f}^{\dagger}_{i\alpha}\hat{f}_{i\alpha}$, respectively. For computational convenience, we have introduced different chemical potentials $\mu_d^A$ and $\mu_d^B$ for different sublattices, which allows us to work with a fixed order parameter, rather than iterating the DMFT equations to determine the

order parameter (which is subject to critical slowing down near $T_c$). The system achieves its initial thermal equilibrium state when the chemical potential is uniform throughout the lattice ($\mu_d^A = \mu_d^B$ and $\mu_f^A = \mu_f^B$). These chemical potentials remain fixed when the external electric field is turned on.

Interaction with the external field in Eq. (2.9) results in a Peierls' substitution to the kinetic term of the Hamiltonian. Hence, the time dependence of the Hamiltonian depends solely on the time-dependent vector potential as follows:

$$t_{ij}^{\alpha\beta}(t) = t_{ij}^{\alpha\beta} \exp\left(-\frac{ie}{hc}\int\limits_{\mathbf{R}_{i,\alpha}}^{\mathbf{R}_{j,\beta}} \mathbf{A}(t)d\mathbf{r}\right), \tag{2.12}$$

where $t_{ij}^{\alpha\beta}$ is the noninteracting hopping matrix.

In the sublattice representation $(A, B)$, the local part of the Hamiltonian is diagonal and the non-local kinetic one is off-diagonal in the case of the nearest-neighbor hopping. In the reduced BZ representation $(1, 2)$ it is *vice versa*: the non-local kinetic part is diagonal and the local interaction $U$-term is off-diagonal.

The Fourier transformation to the momentum space gives the time-dependent kinetic term in the form

$$\begin{aligned}\hat{\mathcal{H}}_{kin}(t) &= \sum_k \begin{bmatrix} c_{\mathbf{k}A}^\dagger & c_{\mathbf{k}B}^\dagger \end{bmatrix} \hat{\epsilon}(\mathbf{k} - e\mathbf{A}(t)) \begin{bmatrix} c_{\mathbf{k}A} \\ c_{\mathbf{k}B} \end{bmatrix} \\ &= \sum_k \begin{bmatrix} \tilde{c}_{1\mathbf{k}}^\dagger & \tilde{c}_{2\mathbf{k}}^\dagger \end{bmatrix} \hat{\tilde{\epsilon}}(\mathbf{k} - e\mathbf{A}(t)) \begin{bmatrix} \tilde{c}_{1\mathbf{k}} \\ \tilde{c}_{2\mathbf{k}} \end{bmatrix}, \end{aligned} \tag{2.13}$$

with an extended band energy [23] whose matrix form in the $(A, B)$ basis becomes

$$\hat{\epsilon}(\mathbf{k} - e\mathbf{A}(t)) = \begin{Vmatrix} 0 & \epsilon(\mathbf{k})\cos(eA(t)) + \bar{\epsilon}(\mathbf{k})\sin(eA(t)) \\ \epsilon(\mathbf{k})\cos(eA(t)) + \bar{\epsilon}(\mathbf{k})\sin(eA(t)) & 0 \end{Vmatrix} \tag{2.14}$$

and performing the unitary transformation in Eq. (2.5), we get the following expression in the reduced BZ representation $(1, 2)$:

$$\hat{\tilde{\epsilon}}(\mathbf{k} - e\mathbf{A}(t)) = \hat{U}\hat{\epsilon}(\mathbf{k} - e\mathbf{A}(t))\hat{U}^{-1} \tag{2.15}$$

$$= \begin{Vmatrix} \epsilon(\mathbf{k})\cos(eA(t)) + \bar{\epsilon}(\mathbf{k})\sin(eA(t)) & 0 \\ 0 & -\epsilon(\mathbf{k})\cos(eA(t)) - \bar{\epsilon}(\mathbf{k})\sin(eA(t)) \end{Vmatrix}.$$



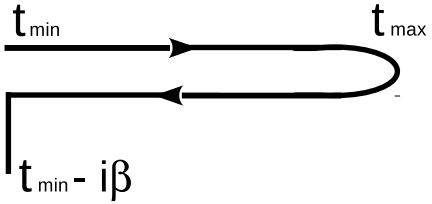


Figure 1. Keldysh-Schwinger contour

Here, we introduced the band energies

$$\epsilon(\mathbf{k}) = \lim_{d\to\infty} \frac{-t^*}{\sqrt{d}} \sum_{r=1}^{d} \cos k_r \quad \text{and} \quad \bar{\epsilon}(\mathbf{k}) = \lim_{d\to\infty} \frac{-t^*}{\sqrt{d}} \sum_{r=1}^{d} \sin k_r$$

and we apply the same scaling of the hopping term as in the equilibrium DMFT.

In the $d \to \infty$ limit the self-energy becomes local and is represented by a diagonal matrix in the sublattice representation. On the other hand, the nonequilibrium noninteracting Green's function is diagonal in the reduced BZ representation and one has to combine these two representations in order to obtain a self-consistent set of DMFT equations in nonequilibrium.

## 3. Real time Green's function in CDW phase

The key object of our interest is the time-dependent Green's function that is defined on the Keldysh-Schwinger contour in Fig. 1:

$$G_{\mathbf{k}}^c(t, t') = -\frac{i}{\hbar}\langle \mathcal{T} c_{\mathbf{k}}(t) c_{\mathbf{k}}^\dagger(t')\rangle. \tag{3.1}$$

We start from the Dyson's equation for the lattice Green's function, which is a $2 \times 2$ matrix equation in the two-sublattice representation $(A, B)$

$$[(i\partial_t{}^c + \mu_d)\hat{I} - \hat{\epsilon}_{\mathbf{k}-e\mathbf{A}(t)}]\hat{G}_{\epsilon,\bar{\epsilon}}^c(t, t') - \int d\bar{t}\hat{\Sigma}^c(t, \bar{t})\hat{G}_{\epsilon,\bar{\epsilon}}^c(\bar{t}, t') = \delta_c(t, t')\hat{I}, \tag{3.2}$$

with the lattice Green's function given by

$$\hat{G}^{c}_{\epsilon,\bar{\epsilon}}(t,t') = \begin{Vmatrix} G^{c,AA}_{\epsilon,\bar{\epsilon}}(t,t') & G^{c,AB}_{\epsilon,\bar{\epsilon}}(t,t') \\ G^{c,BA}_{\epsilon,\bar{\epsilon}}(t,t') & G^{c,BB}_{\epsilon,\bar{\epsilon}}(t,t') \end{Vmatrix} \tag{3.3}$$

and the local self-energy satisfying

$$\hat{\Sigma}^{c}(t,\bar{t}) = \begin{Vmatrix} \Sigma^{c,A}(t,t') & 0 \\ 0 & \Sigma^{c,B}(t,t') \end{Vmatrix}. \tag{3.4}$$

Here $\hat{\epsilon}_{\mathbf{k}-e\mathbf{A}(t)}$ is defined in Eq. (2.14). A formal solution of (3.2) for the Green's function yields

$$\hat{G}^{c}_{\epsilon,\bar{\epsilon}}(t,t') = \left[ (\hat{G}^{c,non}_{\epsilon,\bar{\epsilon}})^{-1} - \hat{\Sigma}^{c} \right]^{-1}(t,t'), \tag{3.5}$$

where the noninteracting Green's function $\hat{G}^{c,non}_{\epsilon,\bar{\epsilon}}(t,t')$ is a solution of the following equation:

$$[(i\partial_t{}^{c} + \mu_d)\hat{I} - \hat{\epsilon}_{\mathbf{k}-e\mathbf{A}(t)}]\hat{G}^{c,non}_{\epsilon,\bar{\epsilon}}(t,t') = \delta_c(t,t')\hat{I}. \tag{3.6}$$

In the two sublattice representation $(A,B)$, the noninteracting Green's function $\hat{G}^{c,non}_{\epsilon,\bar{\epsilon}}(t,t')$ defined by Eq. (3.6) is non-diagonal because the extended band energy $\hat{\epsilon}_{\mathbf{k}-e\mathbf{A}(t)}$ is non-diagonal [see Eq. (2.14)]. On the other hand, in the reduced BZ representation $(1,2)$ the non-interacting Green's function becomes diagonal:

$$\hat{\tilde{G}}^{c,non}_{\epsilon,\bar{\epsilon}}(t,t') = \begin{Vmatrix} G^{c,non}_{\epsilon,\bar{\epsilon}}(t,t') & 0 \\ 0 & G^{c,non}_{-\epsilon,-\bar{\epsilon}}(t,t') \end{Vmatrix}. \tag{3.7}$$

The analytical expression for $G^{c,non}_{\epsilon,\bar{\epsilon}}(t,t')$ is known from the uniform solution [21–23] and is equal to:

$$G^{c,non}_{\epsilon,\bar{\epsilon}}(t,t') = i[f(\epsilon-\mu_d) - \theta_c(t,t')]e^{i\mu(t-t')} \tag{3.8}$$
$$\times \exp\left\{ -i \int_{t'}^{t} d\bar{t} \Big( [\theta(-\bar{t}) + \theta(\bar{t})\cos(eA(\bar{t}))]\epsilon - \theta(\bar{t})\sin(eA(\bar{t}))\bar{\epsilon} \Big) \right\}.$$

Next, we go backward to find the solution for the lattice Green's function from Eq. (3.5) but in the reduced BZ representation. Firstly, applying the unitary transformation in Eq. (2.5) to the self-energy $\hat{\tilde{\Sigma}}^{c}(t,t')$ we find

$$\hat{\tilde{\Sigma}}^{c}(t,\bar{t}) = \hat{U}\hat{\Sigma}^{c}(t,\bar{t})\hat{U}^{-1} \tag{3.9}$$
$$= \frac{1}{2} \begin{Vmatrix} [\Sigma^{c,A} + \Sigma^{c,B}](t,t') & [\Sigma^{c,A} - \Sigma^{c,B}](t,t') \\ [\Sigma^{c,A} - \Sigma^{c,B}](t,t') & [\Sigma^{c,A} + \Sigma^{c,B}](t,t') \end{Vmatrix}.$$

Then, the solution for the lattice Green's function in Eq. (3.5) of the Dyson's equation in Eq. (3.2) becomes [in explicit matrix form on the reduced BZ basis $(1,2)$]

$$\hat{\tilde{G}}^{c}_{\epsilon,\bar{\epsilon}}(t,t') = \begin{Vmatrix} \tilde{G}^{c(1,1)}_{\epsilon,\bar{\epsilon}}(t,t') & \tilde{G}^{c(1,2)}_{\epsilon,\bar{\epsilon}}(t,t') \\ \tilde{G}^{c(2,1)}_{\epsilon,\bar{\epsilon}}(t,t') & \tilde{G}^{c(2,2)}_{\epsilon,\bar{\epsilon}}(t,t') \end{Vmatrix} \tag{3.10}$$
$$= \begin{Vmatrix} (G^{c,non}_{\epsilon,\bar{\epsilon}})^{-1}(t,t') - \frac{\Sigma^{c,A}+\Sigma^{c,B}}{2}(t,t') & -\frac{\Sigma^{c,A}-\Sigma^{c,B}}{2}(t,t') \\ -\frac{\Sigma^{c,A}-\Sigma^{c,B}}{2}(t,t') & (G^{c,non}_{-\epsilon,-\bar{\epsilon}})^{-1}(t,t') - \frac{\Sigma^{c,A}+\Sigma^{c,B}}{2}(t,t') \end{Vmatrix}^{-1}.$$

The Green's functions and self-energies defined on the Keldysh-Schwinger contour are the continuous matrix operators of two time variables. There is no way to handle such an object. Instead, we discretize the contour with a several different grids and then find the continuous matrix limit as an extrapolation onto the limit of zero time discretization using Lagrange's interpolation formula. To find the inverse matrix in Eq. (3.10), where its components are matrices in time variables, we need to apply the block matrix pseudo-inverse formula:

$$\begin{Vmatrix} A & B \\ C & D \end{Vmatrix}^{-1} = \begin{Vmatrix} S_D^{-1} & -A^{-1}BS_A^{-1} \\ -D^{-1}CS_D^{-1} & S_A^{-1} \end{Vmatrix}, \tag{3.11}$$

with $S_A = D - CA^{-1}B$ and $S_D = A - BD^{-1}C$. Using this formula, we derive expressions for the components of the Green's function matrix in the reduced BZ basis $\hat{\tilde{G}}^{c}_{\epsilon,\bar{\epsilon}}(t,t')$ as follows:

$$\tilde{G}^{c(1,1)}_{\epsilon,\bar{\epsilon}}(t,t') =$$
$$= \left\{ (G^{c,non}_{\epsilon,\bar{\epsilon}})^{-1}(t,t') - \frac{\Sigma^{c,A}+\Sigma^{c,B}}{2}(t,t') - \frac{\Sigma^{c,A}-\Sigma^{c,B}}{2}(t,t') \right.$$
$$\left. \times \left[ (G^{c,non}_{-\epsilon,-\bar{\epsilon}})^{-1}(t,t') - \frac{\Sigma^{c,A}+\Sigma^{c,B}}{2}(t,t') \right]^{-1} \frac{\Sigma^{c,A}-\Sigma^{c,B}}{2}(t,t') \right\}^{-1},$$

$$\tilde{G}^{c(2,2)}_{\epsilon,\bar{\epsilon}}(t,t') =$$

$$= \Big\{ (G^{c,non}_{-\epsilon,-\bar{\epsilon}})^{-1}(t,t') - \frac{\Sigma^{c,A}+\Sigma^{c,B}}{2}(t,t') - \frac{\Sigma^{c,A}-\Sigma^{c,B}}{2}(t,t')$$
$$\times \Big[ (G^{c,non}_{\epsilon,\bar{\epsilon}})^{-1}(t,t') - \frac{\Sigma^{c,A}+\Sigma^{c,B}}{2}(t,t') \Big]^{-1} \frac{\Sigma^{c,A}-\Sigma^{c,B}}{2}(t,t') \Big\}^{-1},$$

$$\tilde{G}^{c(1,2)}_{\epsilon,\bar{\epsilon}}(t,t') =$$
$$= \Big\{ (G^{c,non}_{\epsilon,\bar{\epsilon}})^{-1}(t,t') - \frac{\Sigma^{c,A}+\Sigma^{c,B}}{2}(t,t') \Big\}^{-1} \frac{\Sigma^{c,A}-\Sigma^{c,B}}{2} \tilde{G}^{c(2,2)}_{\epsilon,\bar{\epsilon}}(t,t'),$$

$$\tilde{G}^{c(2,1)}_{\epsilon,\bar{\epsilon}}(t,t') =$$
$$= \Big\{ (G^{c,non}_{-\epsilon,-\bar{\epsilon}})^{-1}(t,t') - \frac{\Sigma^{c,A}+\Sigma^{c,B}}{2}(t,t') \Big\}^{-1} \frac{\Sigma^{c,A}-\Sigma^{c,B}}{2} \tilde{G}^{c(1,1)}_{\epsilon,\bar{\epsilon}}(t,t'). \tag{3.12}$$

We have performed a transition onto the reduced BZ basis in order to find the lattice Green's function in terms of the noninteracting Green's function (which is known in momentum representation). Further, we construct the other DMFT equations to make the system of equations self-consistent. In our case of a CDW phase, it is more convenient and clear how to do this in the sublattice basis $(A,B)$. Hence, at this point we apply an inverse transformation from Eq. (2.5) onto the sublattice basis and write down an expressions for the components of the lattice Green's function in the $(A,B)$ basis in terms of its components in the reduced BZ basis $(1,2)$

$$\hat{G}^{c}_{\epsilon,\bar{\epsilon}}(t,t') = \hat{U}^{-1}\hat{\tilde{G}}^{c}_{\epsilon,\bar{\epsilon}}(t,t')\hat{U}, \tag{3.13}$$
$$G^{c(A,A)}_{\epsilon,\bar{\epsilon}}(t,t') = \frac{1}{2}\Big( \tilde{G}^{c(1,1)}_{\epsilon,\bar{\epsilon}}(t,t') + \tilde{G}^{c(2,2)}_{\epsilon,\bar{\epsilon}}(t,t') + \tilde{G}^{c(1,2)}_{\epsilon,\bar{\epsilon}}(t,t') + \tilde{G}^{c(2,1)}_{\epsilon,\bar{\epsilon}}(t,t') \Big),$$
$$G^{c(B,B)}_{\epsilon,\bar{\epsilon}}(t,t') = \frac{1}{2}\Big( \tilde{G}^{c(1,1)}_{\epsilon,\bar{\epsilon}}(t,t') + \tilde{G}^{c(2,2)}_{\epsilon,\bar{\epsilon}}(t,t') - \tilde{G}^{c(1,2)}_{\epsilon,\bar{\epsilon}}(t,t') - \tilde{G}^{c(2,1)}_{\epsilon,\bar{\epsilon}}(t,t') \Big),$$
$$G^{c(A,B)}_{\epsilon,\bar{\epsilon}}(t,t') = \frac{1}{2}\Big( \tilde{G}^{c(1,1)}_{\epsilon,\bar{\epsilon}}(t,t') - \tilde{G}^{c(2,2)}_{\epsilon,\bar{\epsilon}}(t,t') + \tilde{G}^{c(2,1)}_{\epsilon,\bar{\epsilon}}(t,t') - \tilde{G}^{c(1,2)}_{\epsilon,\bar{\epsilon}}(t,t') \Big),$$
$$G^{c(B,A)}_{\epsilon,\bar{\epsilon}}(t,t') = \frac{1}{2}\Big( \tilde{G}^{c(1,1)}_{\epsilon,\bar{\epsilon}}(t,t') - \tilde{G}^{c(2,2)}_{\epsilon,\bar{\epsilon}}(t,t')$$



$$+ \tilde{G}^{c(1,2)}_{\epsilon,\bar{\epsilon}}(t,t') - \tilde{G}^{c(2,1)}_{\epsilon,\bar{\epsilon}}(t,t') \Big),$$

The next step in the DMFT approach is to find the local Green's function, which is further mapped onto a single impurity problem. Since we are considering the two-sublattice system, we have two local Green's functions for the $A$ and $B$ sublattices, respectively.

To calculate the local Green's functions, we need to sum over the reduced BZ all $(\mathbf{k}-\mathbf{eA}(\mathbf{t}))$-dependent functions. Because of presence of the time-depended vector potential, this is not a straightforward procedure. Instead, one has to replace the summation over the BZ by a double integration over the energies $\epsilon$ and $\bar{\epsilon}$

$$\hat{G}^{c}_{loc}(t,t') = \frac{1}{N}\sum_{\mathbf{k}} \hat{G}^{c}_{\mathbf{k}}(t,t') = \int d\epsilon \int d\bar{\epsilon}\rho(\epsilon,\bar{\epsilon})\hat{G}^{c}_{\epsilon,\bar{\epsilon}}(t,t')$$
$$= \left\| \begin{matrix} G^{c,A}_{loc}(t,t') & 0 \\ 0 & G^{c,B}_{loc}(t,t') \end{matrix} \right\|, \tag{3.14}$$

with a joint density of states which is a Gaussian in each variable for the hypercubic lattice [23] and is given by

$$\rho(\epsilon,\bar{\epsilon}) = \frac{1}{\pi}\exp(-\epsilon^2-\bar{\epsilon}^2).$$

Substitution of the components from Eq. (3.13) into Eq. (3.14) results in an expression for the components of the local Green's function for each sublattice as follows:

$$G^{c,A}_{loc}(t,t') =$$
$$= \frac{1}{2}\Big[ \int\int d\epsilon d\bar{\epsilon}\rho(\epsilon,\bar{\epsilon})\tilde{G}^{c(1,1)}_{\epsilon,\bar{\epsilon}}(t,t') + \int\int d\epsilon d\bar{\epsilon}\rho(\epsilon,\bar{\epsilon})\tilde{G}^{c(2,2)}_{\epsilon,\bar{\epsilon}}(t,t')$$
$$+ \int\int d\epsilon d\bar{\epsilon}\rho(\epsilon,\bar{\epsilon})\tilde{G}^{c(1,2)}_{\epsilon,\bar{\epsilon}}(t,t') + \int\int d\epsilon d\bar{\epsilon}\rho(\epsilon,\bar{\epsilon})\tilde{G}^{c(2,1)}_{\epsilon,\bar{\epsilon}}(t,t') \Big]$$
$$= \left[ \begin{matrix} \text{formal change} \quad \epsilon\to-\epsilon', \bar{\epsilon}\to-\bar{\epsilon}' \quad \text{in 2nd and 3rd terms} \\ \text{gives} \quad \tilde{G}^{c(2,2)}_{\epsilon,\bar{\epsilon}} = \tilde{G}^{c(1,1)}_{\epsilon',\bar{\epsilon}'}, \qquad \tilde{G}^{c(1,2)}_{\epsilon,\bar{\epsilon}} = \tilde{G}^{c(2,1)}_{\epsilon',\bar{\epsilon}'}, \\ d\epsilon d\bar{\epsilon} = d\epsilon' d\bar{\epsilon}', \rho(\epsilon,\bar{\epsilon}) = \rho(\epsilon',\bar{\epsilon}') \qquad (\text{see (3.12)}) \end{matrix} \right]$$
$$= \int\int d\epsilon d\bar{\epsilon}\rho(\epsilon,\bar{\epsilon})[I+\Lambda\Sigma][I-K\Sigma\Lambda\Sigma]^{-1}K, \tag{3.15}$$

$$G^{c,B}_{loc}(t,t') = \int\int d\epsilon d\bar{\epsilon}\rho(\epsilon,\bar{\epsilon})[I-\Lambda\Sigma][I-K\Sigma\Lambda\Sigma]^{-1}K,$$

where we introduced new quantities $K$, $\Lambda$, and $\Sigma$, which satisfy

$$K = \left\{(G^{c,non}_{\epsilon,\bar{\epsilon}})^{-1}(t,t') - \frac{\Sigma^{c,A}+\Sigma^{c,B}}{2}(t,t')\right\}^{-1},$$
$$\Lambda = \left\{(G^{c,non}_{-\epsilon,-\bar{\epsilon}})^{-1}(t,t') - \frac{\Sigma^{c,A}+\Sigma^{c,B}}{2}(t,t')\right\}^{-1},$$
$$\Sigma = \frac{\Sigma^{c,A}-\Sigma^{c,B}}{2}(t,t'). \qquad (3.16)$$

One can notice, that in the case where the CDW order vanishes, which implies that $\Sigma^{c,A}(t,t') = \Sigma^{c,B}(t,t') = \Sigma^{c}(t,t')$, the above formulas are reduced to the known result for the uniform phase $G^{c,A}_{loc}(t,t') = G^{c,B}_{loc}(t,t') = G^{c}_{loc}(t,t') = \int\int d\epsilon d\bar{\epsilon}\rho(\epsilon,\bar{\epsilon})\{(G^{c,non}_{\epsilon,\bar{\epsilon}})^{-1}(t,t') - \Sigma^{c}(t,t')\}^{-1}$.

Now, according to the nonequilibrium DMFT procedure [22], we need to map the local lattice Green's function onto the impurity Green's function. Employing Dyson's equation, we introduce an effective medium $\hat{G}^{c}_{0}(t,t')$ by:

$$\hat{G}^{c}_{loc}(t,t') = [(\hat{G}^{c}_{0}(t,t'))^{-1}(t,t') - \hat{\Sigma}^{c}(t,t')]^{-1} = \hat{G}^{c}_{imp}(t,t'). \qquad (3.17)$$

The effective medium $\hat{G}^{c}_{0}(t,t')$ is diagonal in the sublattice representation and its components are equal to

$$G^{c,A}_{0}(t,t') = [(G^{c,A}_{loc})^{-1}(t,t') + \Sigma^{c,A}(t,t')]^{-1},$$
$$G^{c,B}_{0}(t,t') = [(G^{c,B}_{loc})^{-1}(t,t') + \Sigma^{c,B}(t,t')]^{-1}. \qquad (3.18)$$

On the other hand, the effective medium $\hat{G}^{c}_{0}(t,t')$ can be found from the Dyson's equation that defines an effective dynamical mean field $\hat{\lambda}^{c}(t,t')$:

$$(i\partial_t{}^{c} + \mu_d)\hat{G}^{c}_{0}(t,t') - \int d\bar{t}\hat{\lambda}^{c}(t,\bar{t})\hat{G}^{c}_{0}(\bar{t},t') = \delta_c(t,t')\hat{I}. \qquad (3.19)$$

Its components for each sublattice are as follows:

$$G^{c,A}_{0}(t,t') = [(i\partial_t{}^{c} + \mu_d)\delta_c(t,t') - \lambda^{c,A}(t,t')]^{-1},$$
$$G^{c,B}_{0}(t,t') = [(i\partial_t{}^{c} + \mu_d)\delta_c(t,t') - \lambda^{c,B}(t,t')]^{-1}. \qquad (3.20)$$



We next extract the dynamical mean fields for each sublattice

$$\begin{aligned}\lambda^{c,A}(t,t') &= (i\partial_t{}^{c} + \mu_d)\delta_c(t,t') - (G^{c,A}_{0})^{-1}(t,t') \\ &= (i\partial_t{}^{c} + \mu_d)\delta_c(t,t') - (G^{c,A}_{loc})^{-1}(t,t') - \Sigma^{c,A}(t,t'), \\ \lambda^{c,B}(t,t') &= (i\partial_t{}^{c} + \mu_d)\delta_c(t,t') - (G^{c,B}_{0})^{-1}(t,t') \\ &= (i\partial_t{}^{c} + \mu_d)\delta_c(t,t') - (G^{c,B}_{loc})^{-1}(t,t') - \Sigma^{c,B}(t,t'), \qquad (3.21)\end{aligned}$$

which are the effective fields for the nonequilibrium single-impurity problems.

Now, we can close the system of DMFT equations with the solution of the impurity problem. The Falicov-Kimball model has an exact result and for the two sublattice system, we have two solutions for the impurity Green's functions:

$$G^{c,A}_{imp}(t,t') = (1-n^{A}_{f})G^{c,A}_{0}(t,t') + n^{A}_{f}G^{c,A}_{1}(t,t'),$$
$$G^{c,B}_{imp}(t,t') = (1-n^{B}_{f})G^{c,B}_{0}(t,t') + n^{B}_{f}G^{c,B}_{1}(t,t'), \qquad (3.22)$$

where

$$G^{c,\alpha}_{1}(t,t') = [1-G^{c,\alpha}_{0}(t,t')U]^{-1}G^{c,\alpha}_{0}(t,t'), \quad \alpha = A,B. \qquad (3.23)$$

The difference between the $A$ and $B$ sublattices is defined by the order parameter $\Delta n_f$, which is equal to the difference of the $f$-particle occupations at different sublattices ($\Delta n_f = n^{A}_{f} - n^{B}_{f}$). In the CDW phase, the total concentration of localized electrons is fixed $n^{A}_{f} + n^{B}_{f}$ =const, and the order parameter $\Delta n_f$ is defined from the equilibrium condition on the sublattice chemical potentials: $\mu^{A}_{f} - \mu^{B}_{f} = 0$. In nonequilibrium, the order parameter remains the same as in equilibrium because the $f$-particles of the Falicov-Kimball model do not interact with an external time-dependent field and are the conserved quantities in the nonequilibrium case too.

Hence, we may summarize the steps of the nonequilibrium DMFT algorithm. First, we solve the equilibrium problem for the given values of the interaction parameters and temperature. This then determines the order parameter value $\Delta n_f = n^{A}_{f} - n^{B}_{f}$. Then we choose equilibrium results for $\Sigma^{A}_{eq}$ and $\Sigma^{B}_{eq}$ as the initial guess for the nonequilibrium self-energy. Second, we define $G^{c,non}_{\epsilon,\bar{\epsilon}}(t,t')$ and $G^{c,non}_{-\epsilon,-\bar{\epsilon}}(t,t')$, and then calculate the local Green's functions $G^{c,A}_{loc}(t,t')$ and $G^{c,B}_{loc}(t,t')$ as in Eq. (3.15). Third, we define the dynamical mean fields $\lambda^{c,A}(t,t')$ and $\lambda^{c,B}(t,t')$ from Eq. (3.21). Then we calculate the effective mediums $G^{c,A}_{0}(t,t')$, $G^{c,B}_{0}(t,t')$

from Eq. (3.19) and $G_1^{c,A}(t,t')$, $G_1^{c,B}(t,t')$ from Eq. (3.23). Fourth, we define the impurity Green's functions $G_{imp}^{c,A}(t,t')$ and $G_{imp}^{c,B}(t,t')$ from Eq. (3.22). Finally, we set $\hat{G}_{loc}^{c}(t,t') = \hat{G}_{imp}^{c,A}(t,t')$ and extract a new self-energy $\hat{\Sigma}^{c}(t,t')$ from Eq. (3.21). We repeat iterations until we reach the desired accuracy.

## 4. Summary

In this work, we have described the details of the nonequilibrium DMFT procedure in the case of a CDW chess-board phase of the Falicov-Kimbal model. We have derived analytical expressions for the time-dependent lattice Green's functions defined on the Keldysh-Schwinger time contour. We employed the results obtained in paramagnetic phase [22, 23] and generalized them onto a two-sublattice case. Our goal was to present a complete example of the solved problem in the nonequilibrium and ordered phase cases. That is why we have chosen the Falicov-Kimball model. But our results remain general for any other Hubbard-like model if the associated impurity problems can also be solved. Also, we have studied the simplest time dependence of the external field, but this does not affect our derivation. There are other examples of an external field, dictated mainly by the experiments (preparing of a steady state, pump and probe laser pulses etc.), which can be also treated within this formalism.

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