Construction of analytically tractable mean-field theories for quantum models

I. General formalism with application to the Hubbard model at strong coupling

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Abstract. A general theoretical framework for the construction of maximally complex, yet analytically tractable mean-field theories for quantum-mechanical models is presented. These mean-field theories fulfil several strict conditions which are derived from analogous theories in classical statistical mechanics. In particular, they are thermodynamically consistent, conserving approximations and provide exact bounds on the free energy of the original model. The formalism is used to construct a mean-field theory for the Hubbard model in the *strong*-coupling limit.

1. Introduction

Theoretical investigations of quantum-mechanical many-body systems are made difficult by the non-trivial algebra needed to describe these systems and their complicated dynamics. This is particularly evident in the case of strongly interacting systems. In the absence of exact methods there is therefore a great need for reliable, controlled approximation schemes. However, even the construction of approximate schemes is a difficult matter in this case. In fact, for quantum-mechanical lattice models with itinerant degrees of freedom even the familiar concept of a mean-field theory (MFT) is considerably more delicate than in the case of most classical systems. In classical statistical mechanics MFTs usually have very comprehensive properties: *(i)* they represent conserving and thermodynamically consistent approximations, i.e. there exists an explicit free energy functional that is valid for the entire range of input parameters, *(ii)* the free energy contains a set of variational parameters which may be used to optimize the energy, *(iii)* the approximations become exact in one or more particular limits, i.e. there exists one (or more) external small parameter which may be used to improve the MFT systematically by expanding around the mean-field solution. One of the best-known classical MFTs with the above properties is the Weiss molecular field theory for the Ising model. It is a prototypical *single-site* theory which becomes exact for infinite-range interaction, as well as in the limit of high spatial dimensions d (or, more generally, for high coordination number Z) [1]. In the latter case the quantity $1/d$ (or $1/Z$) is a small parameter which can be used to improve the MFT systematically. The Weiss MFT contains no unphysical singularities and is diagrammatically controlled.

Itinerant quantum-mechanical models, such as the Hubbard model and its generalizations, are naturally much more complicated than classical, Ising-type models. This is mainly due to the additional energy transfer between the particles. Consequently, the construction of a MFT with the comprehensive properties of the Weiss MFT for the Ising model will necessarily be much more complicated, too. There do exist various useful mean-field-type approximation schemes, e.g. Hartree-Fock, random phase approximation, saddle-point evaluation of path integrals, decoupling of operators etc.. However, none of them provides a reliable, global description of a given model (e.g. the phase diagram or thermodynamics) in the *entire* range of input parameters. In this situation the investigation of itinerant quantum-mechanical models in the limit $d=\infty$ [2, 3] proves to be a very helpful approach. Indeed, the exact solution of such a model in this limit provides, in principle, an ideal MFT, which has all the desired features of a comprehensive MFT discussed above. Unfortunately, for the Hubbard model this solution cannot, at present, be obtained analytically in closed form: while the spatial properties greatly simplify in the limit $d\to\infty$ [2], the energy exchange between particles with a purely local interaction, i.e. the actual dynamics of the system, does not simplify at all [4]. Hence one is led to an effective single-site problem with a highly complicated dynamics [5–10] where the free energy contains infinitely many coupled complex parameters (the self-energies for different Matsubara-frequencies) which all have to be determined self-consistently. In this situation one has to rely on numerical solutions of the $d=\infty$

self-consistency problem; however, they only provide detailed information about the properties of such a MFT at *finite* temperatures [7–9, 11–13]. It would clearly be highly desirable to gain detailed *analytic* insight, too, in particular at low temperatures, since only an analytic theory is able to give a complete picture of the properties and possible singularities of a given model.

In this paper we wish to construct an analytically tractable MFT for general quantum-mechanical lattice models with itinerant degrees of freedom, including Hubbard-type models, with particular emphasis on the strong-coupling limit. For this to be possible it is obviously necessary to approximate the *dynamics* of the particles generated by the interaction in these models. There exists no unique prescription of how to reduce the energy (i.e. frequency) correlations generated by the quantum interaction. We may, however, set up conditions which have to be fulfilled for a MFT to be as comprehensive as possible and still be analytically tractable. As discussed above it appears that, at present, such a MFT cannot have *all* the comprehensive properties of MFTs in classical statistical mechanics listed earlier. Hence we have to reduce our demands, e.g. by limiting the parameter range for which the MFT is supposed to provide reliable results. Here we may take Hartree-Fock theory as a guiding light. Hartree-Fock is a highly useful MFT which has all the properties of a comprehensive MFT listed above, except one: there exists no small *external* parameter (e.g. $1/d$) which may be used to improve the theory globally for all values of the input parameters. By construction Hartree-Fock is based on a product wave function and is thus only reliable in the limit of *weak* interactions and/or *low* densities, where genuine two-particle correlations can be neglected. In fact, Hartree-Fock does not contain the important *atomic* solution (i.e. the limit where only diagonal matrix elements contribute) at all. Nevertheless it provides a rigorous upper bound on the exact ground state energy for all U-values.

So far there does not exist a MFT for itinerant quantum systems which has the properties of Hartree-Fock theory but is *complementary* in its range of applicability, i.e. is valid in the *strong*-coupling limit. It is our intention in this paper to formulate such a theory. For this MFT to have as many comprehensive properties as possible we formulate the following conditions in close analogy to the properties of MFTs in classical statistical mechanics:

1. There must be a free energy functional which yields explicit, thermodynamically consistent results in the entire range of input parameters (e.g. density n, interaction strength U, temperature T, magnetic field H).
2. The theory must have variational character. Hence the model under consideration will be treated on a mean-field level: the spatial properties are evaluated within a self-consistent, single-site approximation, while the dynamics, i.e. the dynamical exchange between particles, is approximated in terms of a few variational energy parameters.
3. The free energy thus obtained must provide exact bounds on the free energy of the original model.
4. It must be possible to expand around the mean-field solution to calculate corrections.

In Sect. 2 we present the general formalism for the construction of variational MFTs based on the decomposition of a Hamiltonian into solvable sub-Hamiltonians. In Sect. 3 this formalism is applied and worked out in detail for the Hubbard model, with particular emphasis on the strong-coupling limit. A MFT is derived which fulfils all four conditions. The results are discussed in Sect. 4. In the following paper a quantitative analysis of this MFT will be presented. We will construct a mean-field phase diagram for the Hubbard model in $d=\infty$ and will evaluate the bounds on the ground state energy.

2. General formalism for the construction of variational mean-field theories

We consider a quantum-mechanical model described by a Hamiltonian $\hat{H}$ which is defined on a Hilbert space $\mathscr{H}$; we assume that, as usual, an exact solution of the problem is not available. Our construction of a comprehensive mean-field-type theory for the problem under consideration is based on a decomposition of $\hat{H}$ into a set of simplified Hamiltonians whose dynamics can be calculated analytically within a self-consistent single-site approximation. The dynamical *exchange* between the simplified subsystems will be approximated on a mean-field level, too, in terms of a few variational ("mean-field") energy parameters. These parameters are determined by optimizing the resulting mean-field energy, i.e. by maximizing or minimizing this energy, depending on whether it provides a lower or an upper bound on the exact energy, respectively.

We first wish to construct a lower bound. For this we write

$$\hat{H}=\sum_{\alpha=1}^{l}\lambda_\alpha\hat{H}_\alpha \tag{1}$$

where λ_α are real numbers and the sub-Hamiltonians $\hat{H}_\alpha$ need not be specified yet. Denoting the free energy functional by

$$F\{\hat{H}\}=-\beta^{-1}\ln \mathrm{Tr}_{\mathscr{H}}\exp\{-\beta\hat{H}\} \tag{2}$$

and constraining the λ_α in (1) to

$$\sum_{\alpha=1}^{l}\lambda_\alpha=1,\quad \lambda_\alpha\geqq 0 \tag{3}$$

the convexity property [14] of F leads to a *lower* bound on $F\{\hat{H}\}$

$$\sum_{\alpha=1}^{l}\lambda_\alpha F\{\hat{H}_\alpha\}\leqq F\{\hat{H}\}. \tag{4}$$

The l.h.s. of (4) becomes a genuine mean-field theory if the $\hat{H}_\alpha$ contain a set of variational ("mean-field") parameters which will be used to maximize the lower bound. The parameters λ_α should be determined in the same way.

To construct an upper bound on $F\{\hat{H}\}$ we use an arbitrary decomposition

$$\hat{H}=\hat{H}_\alpha+\Delta\hat{H}_\alpha,\quad 1\leqq\alpha\leqq l, \tag{5}$$

with $\Delta\hat{H}_\alpha = \hat{H} - \hat{H}_\alpha$. The $\hat{H}_\alpha$ in (5) need not be those chosen in (1). Application of the Gibbs-Bogoliubov inequality yields

$$F\{\hat{H}\} \leqq F\{\hat{H}_\alpha\} + \langle \Delta\hat{H}_\alpha \rangle_\alpha \tag{6}$$

Here the bracket $\langle \ldots \rangle_\alpha$ denotes the average with respect to the weight $\exp\{-\beta\hat{H}_\alpha\}$. Multiplication of (6) with an arbitrary factor $p_\alpha \geqq 0$, $\sum_{\alpha=1}^{l} p_\alpha = 1$, and summation of both sides of the inequality over α then leads to

$$F\{\hat{H}\} \leqq \sum_{\alpha=1}^{l} p_\alpha \left[F\{\hat{H}_\alpha\} + \langle \Delta\hat{H}_\alpha \rangle_\alpha\right]. \tag{7}$$

Equation (7) is a general upper bound on the free energy $F\{\hat{H}\}$ using sub-Hamiltonians $\hat{H}_\alpha$. As in the case of the λ_α in (4) the factors p_α may be used as variational parameters to optimize the bound (7) (i.e. minimize the upper bound).

For the inequalities (4), (7) to be of use at all, it is essential that the exact free energies (or at least the ground-state energies) of the sub-Hamiltonians $\hat{H}_\alpha$ can be obtained analytically (at least in certain limits, e.g. $d \to \infty$, or $\beta \to \infty$ etc.). However, solving only $\hat{H}_\alpha$ means that the energy *exchange* between these sub-Hamiltonians, which is present in the *full* Hamiltonian $\hat{H}$, is neglected, i.e. the full partition function for $\hat{H}$ in (1) is factorized as

$$\mathrm{Tr}\, e^{-\beta\hat{H}} \to \prod_{\alpha=1}^{l} \mathrm{Tr}\, e^{-\beta\lambda_\alpha\hat{H}_\alpha}. \tag{8}$$

The missing energy exchange now has to be implemented on an analytically tractable, approximate level. Namely, it can be simulated by employing a (small) set of variational mean-field parameters which enter $\hat{H}_\alpha$ as external parameters. The latter are determined in such a way that they optimize the bounds in (4) and (7); in this way the parameters become dynamical variables. It is clear that the quality of the approximation obtained thereby depends on the decomposition of $\hat{H}$: on one hand, the sub-Hamiltonians $\hat{H}_\alpha$, should contain as much of the essential physics described by the full Hamiltonian $\hat{H}$ as possible, so that the approximation of the dynamical exchange between them introduces as little an error as possible; on the other hand the sub-Hamiltonians have to be analytically solvable within a self-consistent single-site approximation (e.g. in $d = \infty$). Clearly the decomposition depends on the Hamiltonian under consideration.

We note that a suitably parametrized decomposition of $\hat{H}$ as in (1), with factorized dynamics (8), indeed fulfils the first three conditions imposed by us on the construction scheme for a MFT. We will now show that it also fulfils the fourth condition, i.e. that it is possible to construct an expansion around the MFT in terms of the perturbation $\Delta\hat{H}_\alpha$ in (6) for all $1 \leqq \alpha \leqq l$. Changing to the interaction picture we define

$$\Delta\hat{H}_\alpha(\tau) \equiv e^{\tau\hat{H}_\alpha}\Delta\hat{H}_\alpha(0)\, e^{-\tau\hat{H}_\alpha} \tag{9}$$

where $0 \leqq \tau \leqq \beta$ and $\Delta\hat{H}_\alpha(0) = \hat{H} - \hat{H}_\alpha$. For the decompositions in (5) the thermodynamic potential $F\{\hat{H}\}$ can then be written exactly as

$$F\{\hat{H}\} = F_{\mathrm{MF}} - \beta^{-1} \sum_{\alpha=1}^{l} p_\alpha \times \ln \left\langle \mathscr{T} \exp\left\{-\int_0^\beta \mathrm{d}\tau \Delta\hat{H}_\alpha(\tau)\right\}\right\rangle_\alpha, \tag{10}$$

where $F_{\mathrm{MF}} = \sum_{\alpha=1}^{l} p_\alpha F\{\hat{H}_\alpha\}$ and $\mathscr{T}$ is the time-ordering operator on $(0, \beta)$. Although there is no small parameter governing the perturbation expansion of the exponential in (10), there is a dimensionless parameter (still a function of the input parameters) which estimates the leading-order fluctuations around the free energy F_{MF}. This parameter is given by $g_2 = \Delta/|\bar{E}_0|$, where

$$\Delta^2 \equiv \sum_{\alpha=1}^{l} p_\alpha \int_0^\beta \mathrm{d}\tau\, \mathrm{d}\tau' \langle \mathscr{T}(\Delta\hat{H}_\alpha(\tau)\Delta\hat{H}_\alpha(\tau'))\rangle_\alpha \tag{11}$$

is the averaged sum of the square of the perturbations $\Delta\hat{H}_\alpha$ with respect to $\hat{H}_\alpha$, and $\bar{E}_0 \equiv \sum_{\alpha=1}^{l} p_\alpha \langle \hat{H}_\alpha \rangle_\alpha$ is the averaged energy of the unperturbed Hamiltonian. If $g_2 \ll 1$ we expect the dynamics of the unperturbed Hamiltonian to simulate the dynamics of the full Hamiltonian $\hat{H}$ rather well. It should, however, be noted that the expansion of the exponential in (10) is not governed by g_2 alone. Higher-order averaged cumulant products of the perturbation operators $\int_0^\beta \mathrm{d}\tau \Delta\hat{H}_\alpha(\tau)$ determine new parameters, unless the $\hat{H}_\alpha$ are quadratic (non-interacting) Hamiltonians. Hence the smallness of the parameter g_2 cannot generally exclude large fluctuations caused by higher-order cumulants.

3. Mean-field theories for the Hubbard model

We now apply the above scheme to the Hubbard model which, in spite of its very simple structure, implies a highly complicated many-body problem for which an exact solution sofar exists only in $d = 1$ [15]. Using the usual notation the Hamiltonian has the form

$$\hat{H} = -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}_{i\sigma}^{+} \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu \sum_{i,\sigma} \hat{n}_{i\sigma}. \tag{12}$$

As a first application we show that it is quite simple to derive the Hartree-Fock approximation within our scheme. For that purpose we partition $\hat{H}$ into two parts ($l = 2$), one containing the kinetic energy

$$\hat{H}_1 = -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}_{i\sigma}^{+} \hat{c}_{j\sigma} + \sum_{i,\sigma} (v_{i\sigma} - \mu)\hat{n}_{i\sigma} \tag{13a}$$

and the other containing the potential energy

$$\hat{H}_2 = U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \sum_{i,\sigma} v_{i\sigma}\hat{n}_{i\sigma}. \tag{13b}$$

Here $v_{i\sigma}$ represent the set of variational parameters which couple $\hat{H}_1$ and $\hat{H}_2$. They will be determined by minimizing the upper bound (7). Note that in our analysis the Hamiltonian $\hat{H}$ already contains the chemical potential μ; hence the thermodynamic potential $F\{\hat{H}\}$ is, in fact, the grand potential Ω. The parameters p_1 and p_2 entering in (7) can be optimized together with the local potentials $v_{i\sigma}$. It appears that $p_1=1, p_2=0$ always produces the best upper bound since this choice minimizes the entropy. Hence we are left with $\hat{H}_1$, (13a), which is the Hartree-Fock Hamiltonian. Varying the r.h.s. of (7) with respect to $v_{i\sigma}$ leads to $v_{i\sigma}=U\langle\hat{n}_{i-\sigma}\rangle_1$, where $\langle\ldots\rangle_1$ denotes the average in terms of $\hat{H}_1$, i.e. yields the unrestricted Hartree-Fock approximation. For the decomposition (13) the general perturbation expansion (10) reduces to the perturbation expansion in U around the Hartree-Fock ground state. - According to the preceeding section we may also construct a lower bound from (13). Introducing λ_1 and $\lambda_2=1-\lambda_1$ we get

$$\lambda_1\Omega\{\hat{H}_1/\lambda_1\}+\lambda_2\Omega\{\hat{H}_2/\lambda_2\}\leqq\Omega\{\hat{H}\}, \tag{14}$$

where $v_{i\sigma}$ and λ_1 are now determined by maximizing the lower bound (14). It is easy to see that, in contrast to the corresponding upper bound, this lower bound is quite uninteresting (it is not determined by a self-consistency problem for the variational parameters, i.e. $v_{i\sigma}$ is no longer given by the Hartree-Fock potential $U\langle\hat{n}_{i-\sigma}\rangle$). Nevertheless the above derivation verifies the well-known fact that Hartree-Fock theory is a thermodynamically consistent, conserving approximation. On the other hand it does not contain true two-particle correlations and thus becomes essentially meaningless in the strong-coupling limit ($U\to\infty$).

To derive a MFT that is valid in the *strong*-coupling limit the sub-Hamiltonians $\hat{H}_\alpha$ have to be chosen in a more sophisticated way. In particular, we demand that the MFT describes the atomic limit ($t=0$ in (12)) exactly. This implies that the on-site interaction must not be decoupled. The only mean-field single-site approximation known to date which indeed does not decouple the Hubbard interaction *and* leads to an analytically tractable problem is the $d\to\infty$ approach when applied to the Falicov-Kimball model [16, 17, 5, 18]. In this model up and down spins interact via the Hubbard interaction, with one spin species being static. The exact solution of this model [16, 17, 5, 18] allows us to derive a new type of MFT for the Hubbard model in the strong coupling limit which leads to the exact result for the atomic limit ($t=0$ in (12)), indicated by the subscript *"at"*, and to explicit bounds on the free energy of the Hubbard model in $d=\infty$. To this end we partition the Hubbard Hamiltonian as

$$\hat{H}=\sum_\sigma\lambda_\sigma\hat{H}_\sigma+\lambda_{at}\hat{H}_{at}, \tag{15}$$

where

$$\lambda_\sigma\hat{H}_\sigma=-t\sum_{\langle ij\rangle}\hat{c}^+_{i\sigma}\hat{c}_{j\sigma}+\sum_{i\sigma'}\lambda_\sigma(v^\sigma_{i\sigma'}-\mu_\sigma)\hat{n}_{i\sigma}+\lambda_\sigma U\sum_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \tag{16a}$$

$$\lambda_{at}\hat{H}_{at}=\sum_{i,\sigma}\lambda_{at}(v^{at}_{i\sigma}-\mu_\sigma)\hat{n}_{i\sigma}+\lambda_{at}U\sum_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \tag{16b}$$

with

$$\sum_{\sigma'}\lambda_{\sigma'}v^{\sigma'}_{i\sigma}+\lambda_{at}v^{at}_{i\sigma}=0. \tag{16c}$$

The variational parameters $v^{\sigma'}_{i\sigma}$ enter into the theory in the same way as in the Hartree-Fock case: they renormalize the chemical potentials $\mu_\sigma=\mu+\sigma H$ in the respective sub-Hamiltonians. The above partitioning of $\hat{H}$ is a generalization of that first discussed by Langer and Mattis [19] for half-filling, which is obtained from (16) by setting $v^{\sigma'}_{i\sigma}=\lambda_{at}=0, \lambda_\sigma=\frac{1}{2}$. The Langer-Mattis decomposition, where the sub-Hamiltonians are not dynamically linked, provides a lower bound on the ground state energy of the Hubbard model. Valenti et al. [20] recently showed that this bound yields good quantitative results for $d=1, 2$. In the following paper we will demonstrate that, by making use of the self-consistent parameters $v^{\sigma'}_{i\sigma}$ in (16), these lower bounds can be substantially improved.

Setting $t=t^*/\sqrt{2d}$ in (16), with $t^*\equiv 1$, to obtain a non-trivial $d\to\infty$ limit [2] the grand potential Ω is a function of U, T and $\mu_\uparrow, \mu_\downarrow$. Using the inequalities (4) and (7) we obtain

$$\begin{aligned}\Omega^\lambda_{\mathrm{MF}}&\equiv\sum_\alpha\Omega_\alpha(\lambda_\alpha U,\lambda_\alpha T,\lambda_\alpha\mu_{\alpha,\uparrow},\lambda_\alpha\mu_{\alpha,\downarrow})\\&\leqq\Omega(U,T,\mu_\uparrow,\mu_\downarrow)\\&\leqq\sum_\alpha p_\alpha\left[1+\sum_\sigma(\mu_\sigma-\mu_{\alpha,\sigma})\frac{\partial}{\partial\mu_{\alpha,\sigma}}\right]\\&\quad\times\Omega_\alpha(U,T,\mu_{\alpha\uparrow},\mu_{\alpha\downarrow}),\end{aligned} \tag{17}$$

where $\alpha=\sigma$, *at* such that $\sum_\alpha p_\alpha=1, p_\alpha\geqq 0$. The r.h.s. of (7) was rewritten using the generating derivatives $\partial/\partial\mu_{\alpha,\sigma}$, with $\mu_{\alpha,\sigma}\equiv\mu_\sigma-v^\alpha_{i\sigma}$, and Ω_σ is the exact grand potential of the Falicov-Kimball model with mobile σ-spins and static $(-\sigma)$-spins. The inequality (17) is valid in any dimension d and represents the most general lower and upper bounds on the free energy (grand potential) of the Hubbard model in terms of the decomposition (16). Note that the upper bound in (17) is a Legendre transform of Ω_α, changing the variational parameters from energy variables $v^\alpha_{i\sigma}$ to their conjugates, the particle densities $n_{\alpha,\sigma}$.

Direct calculation (or a simple argument concerning minimum entropy) shows that the optimal upper bound is obtained for $p_\sigma=1, p_{-\sigma}=p_{at}=0$. The upper bound does not depend on $v^{\sigma'}_{i\sigma}$ at all in this case and is simply provided by the grand potential of the Falicov-Kimball model itself. Hence there is no dynamical coupling between the sub-Hamiltonians. According to our conditions on the properties of a MFT presented in Sect. 1 the free energy functional on the r.h.s. of (17), giving the upper bound, therefore does not provide a MFT for the Hubbard model. Only the free energy functional on the l.h.s. of (17), providing the *lower* bound, may be used for the construction of a MFT for the Hubbard model based on the Falicov-Kimball model. (Note that this is symptomatic for the construction of lower and upper bounds from a particular decomposition of a Hamiltonian: only *one* of the bounds is non-trivial, i.e. self-consistent).

According to our criteria for the construction of a MFT we will now evaluate the free energy functional Ω_σ in a single-site approximation. Since we wish to describe the strong-coupling limit a decoupling of the Hubbard interaction is not permitted. Therefore we employ the exact solution of $\hat{H}_\sigma$ in $d=\infty$ which has been derived only recently [16, 17, 5, 18]. In the absence of a broken spatial symmetry, such that $v_{i\sigma}^{\alpha} \equiv E_\sigma^\alpha$, the explicit result for $\Omega_\uparrow$ is given by [5]

$$
\begin{aligned}
&L^{-1}\Omega_\uparrow(U,T,\mu_{\uparrow,\uparrow},\mu_{\uparrow,\downarrow}) \\
&=\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega f(\omega)\left\{\int_{-\infty}^{\infty} dE\rho_\infty(E)\right. \\
&\quad\times \operatorname{Im}\ln[\omega+\mu_{\uparrow,\uparrow}-\Sigma_\uparrow(\omega)-E+i0^+] \\
&\quad\left.+\operatorname{Im}\ln[1+G_\uparrow(\omega)\Sigma_\uparrow(\omega)]\right\} \\
&\quad-\beta^{-1}\ln[1+\exp\{\beta(\mu_{\uparrow,\downarrow}-\mathscr{E}_\uparrow)\}],
\end{aligned}
\tag{18a}
$$

where L is the number of lattice sites,

$$
\mathscr{E}_\uparrow=\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega f(\omega)\operatorname{Im}\ln\left(1-\frac{UG_\uparrow(\omega)}{1+G_\uparrow(\omega)\Sigma_\uparrow(\omega)}\right) \tag{18b}
$$

is a shift of the atomic $\downarrow$-spin energy level with $f(\omega)=[\exp(\beta\omega)+1]^{-1}$, and $G_\uparrow(\omega)$ and $\Sigma_\uparrow(\omega)$ are frequency-dependent, complex functions which must satisfy the stationarity equations [10]

$$
\frac{\delta\Omega_\uparrow}{\delta G_\uparrow(\omega)}=\frac{\delta\Omega_\uparrow}{\delta\Sigma_\uparrow(\omega)}=0. \tag{19}
$$

Physically, $G_\uparrow(\omega)$ and $\Sigma_\uparrow(\omega)$ represent the local part of the one-electron Green function and the self-energy, respectively. The potential $\Omega_\downarrow$ is then determined analogously and the grand potential for the atomic problem is given by

$$
\begin{aligned}
&\Omega_{at}(U,T,\mu_{at,\uparrow},\mu_{at,\downarrow}) \\
&\quad=-\beta^{-1}\ln(1+e^{\beta\mu_{at,\uparrow}}+e^{\beta\mu_{at,\downarrow}}+e^{\beta(\mu_{at,\uparrow}+\mu_{at,\downarrow}-U)}).
\end{aligned}
\tag{20}
$$

The quantities $\mu_{\alpha,\sigma}=\mu_\sigma-E_\sigma^\alpha$ are appropriately shifted chemical potentials with a constraint on E_σ^α

$$
\sum_{\sigma'}\lambda_{\sigma'}E_\sigma^{\sigma'}+\lambda_{at}E_\sigma^{at}=0,\ \sum_\sigma\lambda_\sigma+\lambda_{at}=1. \tag{21}
$$

Hence there are three sets of independent variational parameters: $\lambda_\sigma, E_\sigma^\uparrow$ and $E_\sigma^\downarrow$. Keeping them fixed as external parameters the grand potentials $\Omega_\uparrow, \Omega_\downarrow$ and Ω_{at} are mutually independent, i.e. the partition function of the Hubbard model is factorized via (8). In this case the subsystems are dynamically decoupled. In particular, there is no energy transfer between them. The missing exchange is now introduced on an approximate level, i.e. variationally, by allowing $E_\sigma^{\sigma'}$ and λ_σ to vary. By maximizing the lower bound in (17) these parameters establish an energetic balance between the sub-systems whereby an effective energy flow is generated. The parameters λ_σ, $E_\sigma^{\sigma'}$ are then no longer external parameters, but *dynamical* variables, which depend on U, T, μ and H. Hence we arrive at the following general mean-field free energy functional for the Hubbard model based on the solution of the Falicov-Kimball model in $d=\infty$:

$$
\begin{aligned}
&L^{-1}\Omega_{\mathrm{MF}}^\lambda(U,T,\mu_\uparrow,\mu_\downarrow;\lambda_\sigma;E_\sigma^{\sigma'})=\sum_\sigma\left\{\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega f_{\lambda_\sigma}(\omega)\right. \\
&\quad\times\left[\int_{-\infty}^{\infty} dE\rho(E)\operatorname{Im}\ln[\omega+\lambda_\sigma(\mu_\sigma-E_\sigma^\sigma)-\Sigma_\sigma(\omega)\right. \\
&\quad\left.-E+i0^+]+\operatorname{Im}\ln[1+G_\sigma(\omega)\Sigma_\sigma(\omega)]\right] \\
&\quad\left.-\lambda_\sigma\beta^{-1}\ln[1+\exp\{\beta((\mu_{-\sigma}-E_{-\sigma}^\sigma)-\mathscr{E}_\sigma/\lambda_\sigma)\}]\right\} \\
&\quad-(1-\lambda_\uparrow-\lambda_\downarrow)\beta^{-1} \\
&\quad\times\ln\left[1+\sum_\sigma\exp\left\{\beta\left(\mu_\sigma+\frac{\lambda_\uparrow E_\sigma^\uparrow+\lambda_\downarrow E_\sigma^\downarrow}{1-\lambda_\uparrow-\lambda_\downarrow}\right)\right\}\right. \\
&\quad\left.+\exp\left\{\beta\left(\sum_\sigma\left(\mu_\sigma+\frac{\lambda_\uparrow E_\sigma^\uparrow+\lambda_\downarrow E_\sigma^\downarrow}{1-\lambda_\uparrow-\lambda_\downarrow}\right)-U\right)\right\}\right],
\end{aligned}
\tag{22a}
$$

where

$$
\mathscr{E}_\sigma=\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega f_{\lambda_\sigma}(\omega)\operatorname{Im}\ln\left(1-\frac{\lambda_\sigma UG_\sigma(\omega)}{1+G_\sigma(\omega)\Sigma_\sigma(\omega)}\right) \tag{22b}
$$

and $f_{\lambda_\sigma}(\omega)=[\exp(\beta\omega/\lambda_\sigma)+1]^{-1}$. The free energy functional $\Omega_{\mathrm{MF}}^\lambda$ is stationary with respect to variations Σ_σ and G_σ, i.e.

$$
\frac{\delta\Omega_{\mathrm{MF}}^\lambda}{\delta\Sigma_\sigma(\omega)}=\frac{\delta\Omega_{\mathrm{MF}}^\lambda}{\delta G_\sigma(\omega)}=0 \tag{23}
$$

and *maximal* with respect to variations of λ_σ and $E_\sigma^{\sigma'}$, i.e.

$$
\frac{\partial\Omega_{\mathrm{MF}}^\lambda}{\partial\lambda_\sigma}=\frac{\partial\Omega_{\mathrm{MF}}^\lambda}{\partial E_\sigma^{\sigma'}}=0 \tag{24}
$$

with the stability condition

$$
\nabla_{\{\lambda,E\}}^2\Omega_{\mathrm{MF}}^\lambda\leqq 0. \tag{25}
$$

The nabla operator $\nabla_{\{\lambda,E\}}$ denotes the total differential with respect to the λ and E variables. Hence we obtain the following inequality for the exact grand potential Ω of the Hubbard model in $d=\infty$

$$
\Omega_{\mathrm{MF}}^\lambda\leqq\Omega\leqq\Omega_\sigma. \tag{26}
$$

For $T=0$ and $n=1$ the lower and upper bound on the free energy of the Hubbard model in (17) are found to coincide, i.e. reduce to zero, when the expectation value of the Hubbard interaction (the density of doubly occupied sites) in the Falicov-Kimball model is zero. This can strictly be true only in the limit $U\to\infty$, in which case it is a rather trivial result. However, if a Brinkman-Rice-

type metal-insulator transition [21] could occur in the ground state (i.e. a transition from a paramagnetic metal to a paramagnetic insulator with ground state energy $E_g = 0$ at a *finite* U) the bounds would coincide, too, and the transition would be described *exactly* by the Falicov-Kimball model.

The MFT described by (22)–(25) is a generalization of a MFT proposed recently by us [10]. The latter can be obtained from the above expressions by formally setting $\lambda_\sigma = 1$, $\lambda_{at} = -1$. In principle the resulting free energy expression will then no longer provide a lower bound on the free energy of the Hubbard model since, according to (3), this requires all λ to be positive. However, we will see that in the *ground state* the free energy derived by us in [10] may be expressed in terms of $\Omega^{\lambda}_{\mathrm{MF}}$ in (22) and hence provides a lower bound after all. Using $\lambda_\sigma = 1$, $\lambda_{at} = -1$ or, equivalently, $p_\sigma = 1$ and $p_{at} = -1$ in (10) we are led to the exact expression for the grand potential of the Hubbard model

$$\Omega(U, T, \mu_\uparrow, \mu_\downarrow) = \Omega_{\mathrm{MF}}(U, T, \mu_\uparrow, \mu_\downarrow; E^I_\sigma, E^L_\sigma) - \beta^{-1} \sum_\alpha p_\alpha \ln \left\langle \mathscr{T} \exp\left\{ -\int_0^\beta \mathrm{d}\tau \Delta \hat{H}_\alpha(\tau) \right\} \right\rangle_\alpha \tag{27}$$

where again $\alpha = \sigma, at$, with

$$\Delta \hat{H}_\sigma(\tau) = -t \sum_{\langle ij \rangle} \hat{c}^+_{i-\sigma}(\tau) \hat{c}_{j-\sigma}(\tau) + \sum_i [(E^I_{-\sigma} - E^L_{-\sigma}) \hat{n}_{i-\sigma}(\tau) - E^I_\sigma \hat{n}_{i\sigma}(\tau)] \tag{28a}$$

and

$$\Delta \hat{H}_{at}(\tau) = -t \sum_{\langle ij \rangle, \sigma} \hat{c}^+_{i\sigma}(\tau) \hat{c}_{j\sigma}(\tau) - \sum_{i,\sigma} E^L_\sigma \hat{n}_{i\sigma}(\tau). \tag{28b}$$

Here we used the notation $E^I_\sigma \equiv E^\sigma_\sigma$ and $E^L_\sigma \equiv E^{at}_\sigma$ where E^I_σ parametrizes the mean energy transfer between mobile ("*I*tinerant") and fixed spins, while E^L_σ describes the effective mean-field energy of the fixed ("*L*ocalized") σ-spins [10]. The grand potential Ω_{MF} is precisely the mean-field grand potential derived in [10]. The expansion in (27) represents a renormalized expansion in the hopping amplitude.

At $T = 0$ we easily find that Ω_{MF} and $\Omega^{\lambda}_{\mathrm{MF}}$, (22), are related by

$$\Omega_{\mathrm{MF}}(U/2, 0, \mu_\uparrow/2, \mu_\downarrow/2; E^I_\sigma, E^L_\sigma) = \Omega^{\lambda}_{\mathrm{MF}}(U, 0, \mu_\uparrow, \mu_\downarrow; \lambda_\sigma = 1/2; E^I_\sigma, E^L_\sigma). \tag{29}$$

Hence the variational character of the mean-field grand potential Ω_{MF} remains, at least at $T = 0$. As discussed in ref. [10] Ω_{MF} defines a thermodynamically consistent, conserving, diagrammatically controlled MFT. Its construction is conceptually similar to that of the well-known Hubbard-III approximation [22] without having the serious deficiencies of the latter [23]. Hence to date Ω_{MF} or, more generally, $\Omega^{\lambda}_{\mathrm{MF}}$ provide the *best* analytically tractable, thermodynamically consistent theory for the Hubbard model that describes the atomic limit exactly. Obviously Ω_{MF} satisfies all four conditions for the construction of a MFT for itinerant quantum systems listed in the Introduction and, in addition, describes the atomic limit correctly. Moreover, the stationarity of Ω_{MF} with respect to $E^{I,L}_\sigma$ has a clear physical meaning: it guarantees that the average number of particles with a given spin σ, n_σ, is identical in all the sub-systems and equal to that of the actual system. Because of this conservation of particle densities we can rewrite the inequalities for the thermodynamic potentials in terms of fixed n_σ instead of fixed μ_σ, i.e. apply them to the free energies F at $T = 0$ as

$$F_{\mathrm{MF}}(U/2, 0, n_\uparrow, n_\downarrow, E^I_\sigma, E^L_\sigma) \leqq F(U, 0, n_\uparrow, n_\downarrow). \tag{30}$$

We thus derived a variational lower bound on the ground state energy of the Hubbard model for fixed band filling, which will be explicitly evaluated in the following paper. Note that the lower bounds generally rescale the interaction strength of the original Hamiltonian; this is a consequence of the convexity property of the thermodynamic potentials [14].

4. Conclusions

In this paper we presented a general formalism for the construction of analytically tractable, mean-field-type theories for quantum Hamiltonians of interacting particles. The method is based on the decomposition of the original Hamiltonian into simpler ones that can be solved within a mean-field, single-site approximation (e.g. in $d = \infty$). The dynamical exchange between the sub-Hamiltonians is then introduced on a variational level in terms of a set of mean-field energy parameters. The construction is motivated by an effort to derive maximally complex, *analytically tractable* MFTs for Hubbard-type Hamiltonians in analogy to the comprehensive MFTs in statistical mechanics. To this end we formulated four "minimal" criteria which any MFT should fulfil. We discussed two MFTs that fit into this scheme. One is the Hartree-Fock approximation which is based on a decomposition into kinetic and potential energy. It provides an upper bound on the free energy of the Hubbard model in any dimension d. However, since Hartree-Fock theory is a self-consistent extrapolation of the non-interacting case its results are no longer reliable at large interactions and it does not contain the atomic limit at all. To construct a MFT for the Hubbard model which has the properties of Hartree-Fock theory and is complementary in its range of applicability, i.e. is valid in the *strong*-coupling limit, and becomes exact in the atomic limit, we used a decomposition of the Hubbard Hamiltonian into self-consistently linked Falicov-Kimball models which were evaluated in $d = \infty$ dimensions. The free energy functional of this MFT can be derived in closed form and provides the sofar best lower bound on the ground state energy of the Hubbard model in $d = \infty$. It is conceptually similar to the well-known Hubbard-III solution but, in contrast to

the latter, is a thermodynamically consistent, diagrammatically controlled theory with exact limits. Quantitative results, i.e. ground state properties and the phase diagram, of this MFT are presented in the following paper.

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