CORRELATED LATTICE ELECTRONS: EXACT MEAN FIELD DESCRIPTION IN INFINITE DIMENSIONS

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It is shown that correlated Fermi systems in high dimensions can be *exactly* described in terms of an effective Hamiltonian with obvious mean field character. The method is applied to, and worked out for, a simplified Hubbard model. Thereby the exact solution in $d = \infty$ is recovered.

It has recently become clear [1] that the limit of high dimensions ($d \to \infty$) is an extremely useful starting point for studying correlated Fermi systems, since their theoretical description becomes simpler in this limit, while remaining non-trivial. Over the past two years, many interesting new results have been found [2-4], but one aspect remained obscure: whether some type of mean field theory becomes exact in $d \to \infty$ or, conversely, whether the exact solution of the model in $d = \infty$ has a mean field character. *That* mean field theory should become exact is, at least, what one would expect on the basis of classical [5] and quantum mechanical [6] spin systems. One result in this direction is easily obtained: the usual "mean field" description based on Hartree-Fock definitely does not become exact in $d = \infty$, [8] since, at weak coupling, the correlation energy for the Hubbard model obtained by Hartree-Fock is non-analytically small, in contrast to the exact result. In this paper it is shown how a mean field description, that does become exact, can be constructed.

Consider the Hubbard model [7], which is a standard model for itinerant magnetism and also for high-T_c-superconductivity. The Hubbard Hamiltonian is in its grand canonical form given by

$$H = H_t + H_U + H_\mu \tag{1a}$$

where

$$H_t = \sum_{\mathbf{ij},\sigma} t_{\mathbf{ij}\sigma} \hat{c}^+_{\mathbf{i}\sigma} \hat{c}_{\mathbf{j}\sigma} \tag{1b}$$

$$H_U = U \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}\uparrow} \hat{n}_{\mathbf{i}\downarrow} \qquad (U > 0) \tag{1c}$$

$$H_\mu = -\sum_{\mathbf{i}\sigma} \mu_\sigma \hat{n}_{\mathbf{i}\sigma} \tag{1d}$$

Here $\hat{c}^+_{\mathbf{i}\sigma}(\hat{c}_{\mathbf{i}\sigma})$ is a creation (annihilation) operator for an electron with spin σ at site $\mathbf{i}$, and $\hat{n}_{\mathbf{i}\sigma} = \hat{c}^+_{\mathbf{i}\sigma}\hat{c}_{\mathbf{i}\sigma}$. In spite of the simplifications occurring in high dimensions [1,2], the Hubbard model has as yet resisted an exact solution. However, very recently the exact solution in $d = \infty$ has been found for a simplified version of the Hubbard model, the so-called Falicov-Kimball model [3], where only one type of electron is mobile. Apart from the deficiencies of Hartree-Fock for the Hubbard model as discussed above, this approximation is also poor for the Falicov-Kimball model, especially at large U, e. g. the predicted critical temperature ($T_c \sim U$) deviates drastically from the exact result [9]: $T_c \sim U^{-1}$.

To construct a Hamiltonian that becomes exact in high dimensions we consider the Falicov-Kimball model. Furthermore the lattice best suited for our analysis is the Bethe lattice. The limit of high dimensions then corresponds to a large coordination number (i. e. $Z \to \infty$). Note that both the Bethe lattice and the hypercubical lattice have AB-structure, so that the thermodynamical properties are essentially the same [9].

Therefore consider the Hamiltonian (1) with $t_{\mathbf{ij}\uparrow} = 0$ and $t_{\mathbf{ij}\downarrow} = -\bar{t}_{\mathbf{ij}}/Z^{1/2}$, where $\bar{t}_{\mathbf{ij}} = 1$ for nearest neighbors and $\bar{t}_{\mathbf{ij}} = 0$ otherwise. The Falicov-Kimball model describes immobile "nuclei" (spin $\uparrow$), interacting via mobile "electrons"(spin $\downarrow$). In view of the discrete symmetry (presence/absence of a nucleus) it is not surprising that the model contains an Ising-like phase transition at half filling [9].

To obtain a mean field description we note that a site $\mathbf{i}$ "sees" its surroundings through Green functions of the form $G(\tau - \tau') = \langle T_\tau \hat{c}_{\mathbf{i}\downarrow}(\tau)\hat{c}^+_{\mathbf{i}\downarrow}(\tau')\rangle$. The time developement of $G(\tau-\tau')$ is described by the equations of motion: the various derivatives $\partial G/\partial\tau$, $\partial^2 G/\partial\tau^2, \ldots$, involve the commutators $[H, c_{\mathbf{i}\downarrow}]$, $[U[H, c_{\mathbf{i}\downarrow}]]$, etc.. The basic point is that these commutators assume a very simple form in the limit $Z \to \infty$. For instance, the commutator $[H, c_{\mathbf{i}\downarrow}]$ can be described in terms of two new fermions, representing the entire first shell of neighbors around site $\mathbf{i}$:

$$\hat{c}_e \equiv [(1-\rho_1)Z]^{-1/2} \sum_{|\mathbf{i}-\mathbf{j}|=1} (1 - \hat{n}_{\mathbf{j}\uparrow})\hat{c}_{\mathbf{j}\downarrow} \tag{2a}$$

$$\hat{c}_f \equiv [\rho_1 Z]^{-1/2} \sum_{|\mathbf{i}-\mathbf{j}|=1} \hat{n}_{\mathbf{j}\uparrow}\hat{c}_{\mathbf{j}\downarrow} \tag{2b}$$

where ρ_1 is the density of nuclei in the first shell. Similarly the commutator $[H, [H, \hat{c}_{\mathbf{i}\downarrow}]]$ introduces four new fermions, and in general the n-th commutator yields 2^n new fermionic variables, corresponding to the 2^n possible ways of finding n sites either occupied or unoccupied by a nucleus. The new fermions are denoted by c_X, where $X = \{x_1, \ldots, x_n\}$ and $x_l = 0, 1$ indicates the absence/presence of a nucleus in the l-th shell around $\mathbf{i}$.

The same commutators can also be derived from an effective Hamiltonian H^{MF} having the same form (1a) as H, but with H_t^{MF}, H_U^{MF} and H_μ^{MF} depending only of c_X:

$$H_U^{MF} = U \hat{n}_{\mathbf{i}\uparrow}\hat{n}_{\mathbf{i}\downarrow} \tag{3a}$$

$$H_t^{MF} = \sum_{l(X)\geq 0} [t_{l+1}^0(\hat{c}_{X0}^+\hat{c}_X + \hat{c}_X^+\hat{c}_{X0}) + t_{l+1}^1(\hat{c}_{X1}^+\hat{c}_X + \hat{c}_X^+\hat{c}_{X1})] \quad (3b)$$

$$H_\mu^{MF} = -\Big\{\mu_\downarrow \hat{n}_{i\downarrow} + \mu_\uparrow \hat{n}_{i\uparrow} + \sum_{l(X)\geq 0} [\mu_\downarrow n_{X0} + (\mu_\downarrow - U)n_{X1}]\Big\} \quad (3c)$$

Here the hopping matrix elements are defined by $t_l^0 \equiv (1-\rho_l)^{1/2}$ and $t_l^1 \equiv \rho_l^{1/2}$, where ρ_l is the density of nuclei in the l-th shell. Furthermore $l(X)$ is the length (number of components) of X, and the notation $X0$ or $X1$ represents the $(l+1)$-dimensional vectors $(X,0)$ or $(X,1)$. Note that H^{MF} has the form of a tight-binding model on a Bethe lattice with coordination number $Z^{MF} = 3$. Also note that: (1) the Hubbard interaction remains only on site **i**; (2) a Hartree-Fock decoupling in H_U^{MF} does not occur, since the correlations between electrons and nuclei on-site **i** are in general not small; (3) H^{MF} depends on the nuclei surrounding site **i** only in an average manner, through the density ρ_l (order parameter). The last point makes clear that H^{MF} is truely a mean field Hamiltonian.

Obviously there are also great differences between the quantum Hamiltonian H^{MF} and classical mean field theory. First, H^{MF} contains many mean fields c_X, representing the various shells around **i**. This feature is due to the hopping. Secondly, the mean fields c_X in (3) are operators, not numbers, which emphasizes the quantum character of the model.

Having identified H^{MF} as a typical mean field reformulation of the original model one may wonder whether the phase transition described by H^{MF} also displays the usual mean field behavior of its order parameter. The order parameter in this case is the density difference Δ of the nuclei on the A- and B-sublattices.

To investigate this question we focus on the half-filled case ($\mu_\uparrow = \mu_\downarrow = U/2$). The Green functions $\langle T_\tau \hat{c}_{i\downarrow}(\tau)\hat{c}_{j\downarrow}^+(\tau')\rangle$, with $\mid \mathbf{i}-\mathbf{j} \mid = 0,1$, can easily be calculated using the standard techniques developed for the Bethe lattice [10]. The assumption that the low temperature phase has AB-structure implies $\rho_{2l-1} = \rho_1$ and $\rho_{2l} = \rho_2 (l = 1,2,\ldots)$, so that the order parameter is $\Delta = \mid \rho_1 - \rho_2 \mid$. The Green functions depend explicitly on the parameter Δ. Knowing the Green functions, we can calculate the kinetic energy per site $e_t(\beta,\Delta)$, the interaction energy $e_U(\beta,\Delta)$, the internal energy $e \equiv e_t + e_U$ and, by integrating the relation $e = \partial\beta f/\partial\beta$, the free energy per site $f(\beta,\Delta)$. The physically realized value of Δ, denoted by $\Delta_0(T)$, is obtained by minimizing the free enegy with respect to Δ.

In order to localized the phase transition, we may expand $f(\beta,\Delta)$ in a power series around $\Delta = 0$. From this expansions the critical temperature $T_c(U)$ can readily be calculated for large and small values of U. One finds that

$$k_B T_c \sim (2U)^{-1} \qquad (U \to \infty) \quad (4a)$$

$$\sim \frac{U^2}{2\pi} ln(U^{-1}) \qquad (U \downarrow 0) \quad (4b)$$

so that T_c vanishes in both limits, as expected.

The temperature dependence of $\Delta_0(T)$ near T_c follows directly by minimizing $f(\beta,\Delta)$ with respect to Δ as

$$\Delta_0(T) \propto (T_c - T)^{1/2} \qquad (T \uparrow T_c) \quad (5)$$

Similarly one finds, by expanding $f(\beta,\Delta)$ in powers of $(1-\Delta)$, that the low temperature behavior of $\Delta_0(T)$ is given by

$$1 - \Delta_0(T) \propto \exp(-C/T) \qquad (T \downarrow 0) \quad (6)$$

where C is some positive constant. Equations (5) and (6) clearly show that the order parameter in this quantum mechanical model is indeed completely analogous to the magnetization of the Ising and Heisenberg models in $d = \infty$, thus stipulating its mean field character.

A more detailed discussion of the model discussed in this paper will be published elsewhere.

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