A partition functional and thermodynamic properties of the infinite-dimensional Hubbard model

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Abstract

An approximate partition functional is derived for the infinite-dimensional Hubbard model. This functional naturally includes the exact solution of the Falicov-Kimball model as a special case, and is exact in the uncorrelated and atomic limits. It explicitly keeps spin-symmetry. For the case of the Lorentzian density of states, we find that the Luttinger theorem is satisfied at zero temperature. The susceptibility crosses over smoothly from that expected for an uncorrelated state with antiferromagnetic fluctuations at high temperature to a correlated state at low temperature via a Kondo-type anomaly at a characteristic temperature $T^\star$. We attribute this anomaly to the appearance of the Hubbard pseudo-gap. The specific heat also shows a peak near $T^\star$. The resistivity goes to zero at zero temperature, in contrast to other approximations, rises sharply around $T^\star$ and has a rough linear temperature dependence above $T^\star$.

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1 Introduction

The single-band Hubbard model (HM) and the periodic Anderson model have attracted a great deal of interest since the heavy fermion and high temperature superconductors were discovered. Although there has been intensive theoretical work on both models, the knowledge we have for them is still limited, with an exact solution known only for the one-dimensional HM [1]. An important advance was made by Metzner and Vollhardt [2], who observed that any diagrammatic treatment of fermion lattice models simplifies in infinite dimensions. The proper self-energy becomes site-diagonal and momentum conservation is thus irrelevant [3]. Despite this simplification, the dynamic properties remain non-trivial. This discovery has stimulated much attention recently [4]. Nearly all the phenomena associated with strong electron correlations have been found in the infinite dimensional models: the Mott transition [5], antiferromagnetism [6], Fermi liquid or non-Fermi liquid behavior [7], and even the possibility of superconductivity [8]. The infinite dimensional models appear to be a good starting point for studying electron correlations.

Brandt and Mielsch [9] first showed that the infinite dimensional \((D^\infty)\) HM can be mapped onto an atomic problem in the presence of two time-dependent external fields. They were able to solve exactly the \(D^\infty\) Falicov-Kimball model, which corresponds to one time-dependent external field. A complete exact solution for the case of two external fields has not been possible. An equivalent mapping to the Anderson impurity model with a self-consistent condition has also been found [10, 3]. This has been used to calculate properties of the \(D^\infty\) HM [5, 6] and periodic Anderson model [11] by the quantum Monte Carlo (QMC) method. Although the QMC method is essentially exact, it can not treat the whole parameter region, in particular the cases of large \(U\) and low temperatures. Analytical continuation using the maximum entropy method to calculate some dynamic quantities is also problematic. A controlled approximate solution is clearly desirable for the whole parameter region.

Many approximate schemes have been developed for the strongly correlated electron systems, such as the alloy analogy approximation (plus coherent potential approximation), equation-of-motion decoupling [12], slave boson [13] and slave fermion [14] approaches, etc.. Unfortunately, they are usually not controlled approximations and do not become exact in physically-relevant limits.

In the present paper we report on a better approximation scheme for the infinite dimensional models. The alloy analogy approximation [12] (as well as the Hubbard-III approximation [15] and higher-order equation-of-motion decoupling [12]) do rather well for high temperatures, and are exact in the free electron and atomic limits. But they violate the Luttinger theorem at \(T = 0\), and do not include magnetic order probably as a result of breaking spin symmetry. The slave-boson and slave-fermion mean-field approximations usually give us contradictory results, and do not become exact even in the limit of free electrons. Our approximation scheme retains the merits of the previous approximations especially at high temperature and respects the spin symmetry explicitly. It satisfies the Luttinger theorem at zero temperature thereby remedying the most serious defect of approximations such as the alloy analogy approximation. Furthermore, the approximate solution is obtained in an expansion scheme so that it
can be improved systematically by including higher-order effects.

Janiš and Vollhardt [17] have already suggested an approximate solution to the $D^\infty$ Hubbard model. Their ansatz for the thermodynamic potential is the linear combination of the potentials for two Falicov-Kimball models obtained by assigning one potential to one spin and retaining the other spin as the impurity. Although this ansatz is formally written to be spin-symmetric, the ingredients they used, i.e. the solution of the Falicov-Kimball model, break the symmetry intrinsically. It does not satisfy the Luttinger theorem at zero temperature.

We use the Brandt-Mielsch mapping [9] to find an approximate solution to the partition functional of the $D^\infty$ HM (including the periodic Anderson model) [18]. From the partition functional one can obtain the self-energy and all the thermodynamic properties of the system as well as some correlation functions. The functional we obtain naturally contains the exact solution of the $D^\infty$ Falicov-Kimball model as a special case, and is exact in the uncorrelated and atomic limits. The spin-symmetry is retained explicitly.

To demonstrate the approximation scheme, we calculate the thermodynamic properties of the $D^\infty$ HM for a Lorentzian density of states (DOS). For this simple DOS, one can obtain some analytic expressions for physical quantities. The main physical properties of the $D^\infty$ HM (except the Mott transition) are expected to remain for this DOS [19]. We find that at zero temperature the system is a Fermi liquid (except at half-filling), which is consistent with the exact result of Georges and Kotliar [10]. The Luttinger theorem is satisfied. As the temperature is increased, the system crosses over continuously from a correlated state to an uncorrelated state with a Curie-Weiss susceptibility via a Kondo-like anomaly. This is in contrast to other approximations in which either the local moment behavior observed at high temperatures or the strongly correlated behavior observed at low temperatures is not properly reproduced [16] [12]. The Kondo-like anomaly here actually results from the Hubbard pseudogap. The specific heat shows a peak at the corresponding (Kondo) characteristic temperature $T^\star$. The resistivity goes to zero at $T = 0$. This is completely different from the result of the alloy analogy approximation and other schemes, which break the Luttinger theorem at zero temperature so that the resistivity always goes up as temperature decreases.

The paper is organized as follows. We briefly outline the main features of the $D^\infty$ HM and the Brandt-Mielsch mapping in Section II. We derive the approximate partition functional by an expansion in Section III. Some physical quantities, such as the susceptibility, the specific heat and the resistivity are then calculated using the functional in Section IV. Finally, we discuss our results in Section V.

2 The infinite-dimensional Hubbard model and equivalent atomic problem
2.1 The $D^\infty$ Hubbard model

The Hubbard Hamiltonian for large dimensions, $D$, is \cite{2}

$$H_H = -\frac{1}{2\sqrt{D}} \sum_{ij} t_{ij} a_{i,\sigma}^\dagger a_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \sum_{i\sigma} (E_\sigma - \mu) a_{i,\sigma}^\dagger a_{i,\sigma}, \quad (1)$$

where $a_{i,\sigma}, a_{i,\sigma}^\dagger$ and $n_{i,\sigma} = a_{i,\sigma}^\dagger a_{i,\sigma}$ are usual fermion operators; $\mu$ is the chemical potential, $E_\sigma$ takes account of the spin-dependence of the atomic levels. In the presence of the external field $h$, $E_\sigma = E_0 - \sigma \mu_B h$ ($\mu_B$ the Bohr magneton). The hopping term is scaled so as to make the kinetic energy and the interaction term competitive.

Because of the scaling by $1/\sqrt{D}$ for the kinetic term in (1), the self-energy becomes site-diagonal \cite{2, 3}, i.e. its Fourier transform $\Sigma(i\omega_n, k) \equiv \Sigma(i\omega_n)$ is a $k$-independent quantity. For a homogeneous system \cite{20}, the Dyson equation for the full momentum-dependent Green’s function of (1) is given by

$$G_\sigma(i\omega_n, k) = [i\omega_n - (E_\sigma - \mu) - \Sigma_\sigma(i\omega_n) - \varepsilon(k)]^{-1}. \quad (2)$$

Integrating $G_\sigma(i\omega_n, k)$ over $k$ gives the following local Green’s function

$$G^{\text{loc}}_\sigma(i\omega_n) \equiv \langle G_\sigma^n(k) \rangle_k = \int_{-\infty}^{\infty} \frac{\rho_0(\varepsilon) d\varepsilon}{i\omega_n - (E_\sigma - \mu) - \Sigma_\sigma(i\omega_n) - \varepsilon}. \quad (3)$$

Here $\rho_0(\varepsilon)$ is the bare density of states (DOS), which is of Gaussian type \cite{2, 3} for the nearest neighbor hopping in (1):

$$\rho_0(\varepsilon) = \sum_k \delta(\varepsilon - \varepsilon_k) = \frac{1}{\sqrt{\pi}} \exp[-\varepsilon^2].$$

The self-energy can be expressed as a functional of the local Green’s functional $G^{\text{loc}}_\sigma(i\omega_n)$, as shown using the perturbation expansion in \cite{21}:

$$\Sigma(i\omega_n) = \Sigma[G^{\text{loc}}_{\sigma}(i\omega_n)]. \quad (4)$$

Once the self-energy functional (4) is known, one can determine the local Green’s function from (3), and, consequently, the self-energy. Eq. (3) therefore provides a self-consistent equation for determining the Green’s function of the system.

2.2 The Brandt-Mielsch mapping

The central problem is to find the self-energy, $\Sigma$, as a functional of the local Green’s function $G^{\text{loc}}_\sigma(i\omega_n)$. Brandt and Mielsch \cite{9} mapped the $D^\infty$ HM onto an atomic problem with two external fields to find this functional.

For an atomic (single site) problem, $H_H$ in (1) reduces to the atomic Hamiltonian $H = H_0 + V$, where

$$H_0 = \sum_\sigma (E_\sigma - \mu) a_{\sigma}^\dagger a_{\sigma},$$
$$V = U n_\uparrow n_\downarrow. \quad (5)$$
Of course, the Hamiltonian $H$ can easily be solved. However, when the two external fields are introduced, the problem is never trivial.

A generating partition functional is defined as

$$Z = \text{Tr}\{e^{-\beta H}S\},$$

where

$$S = T_\tau \exp\{- \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma \lambda^\sigma(\tau, \tau') a^\dagger_\sigma(\tau) a^H_\sigma(\tau')\}$$

with $a^H_\sigma(\tau) = e^{H\tau} a^\dagger_\sigma e^{-H\tau}$ and $\lambda^\sigma(\tau, \tau')$ is an external field. The Green’s function is defined by functional differentiation: $\bar{G}^\sigma(\tau, \tau') = -\delta \ln Z / \delta \lambda^\sigma(\tau', \tau)$. Using Matsubara’s formalism, we write

$$\lambda^\sigma(\tau, \tau') = \frac{1}{\beta} \sum_n \exp[-i\omega_n(\tau - \tau')] \lambda^\sigma_n,$$

where $\omega_n = (2n + 1)\pi/\beta$. The Fourier transform of the Green’s function, $\bar{G}^\sigma(i\omega_n)$, is then given by

$$\bar{G}^\sigma(i\omega_n) = -\partial \ln Z / \partial \lambda^\sigma_n$$

The self-energy is defined via

$$\Sigma^\sigma(i\omega_n) = G^\sigma_0(i\omega_n)^{-1} - \bar{G}^\sigma(i\omega_n)^{-1},$$

where

$$G^\sigma_0(i\omega_n) = [i\omega_n - (E^\sigma - \mu) - \lambda^\sigma_n]^{-1}.$$

One may ask what the relation is between the local Green’s function $G^{\text{loc}}_\sigma(i\omega_n)$ in (3) and the Green’s function $\bar{G}^\sigma(i\omega_n)$ defined in (5). When one expands the self-energy of (1) in a series of skeleton diagrams in terms of $G^\sigma_\sigma(i\omega_n)$, i.e., expands in the formalism of Baym and Kadanoff [22], one finds that there is a one-to-one correspondence between these skeleton diagrams and those of the self-energy of the original Hubbard model in (1) in terms of $G^{\text{loc}}_\sigma(i\omega_n)$. The self-energy (10), when written as a functional of $G^\sigma_\sigma(i\omega_n)$, therefore has the same form as the self-energy functional of the Hubbard model (1). Since this functional is what is inserted in (3), it is clear that $\bar{G}^\sigma(i\omega_n)$ and $G^{\text{loc}}_\sigma(i\omega_n)$ are the same once Eq. (3) has been solved self-consistently.

In a real calculation of the local Green’s function from the self-consistent equation (3), one does not need to find an explicit form of the self-energy as a function of $G^\sigma_\sigma(i\omega_n)$. It is in general easier to determine from (3) the $\lambda^\sigma_n$ (or equivalently the Green’s function $G^\sigma_0(i\omega_n)$ of (10)), and then to use the $\lambda^\sigma_n$ to fix the self-energy in (11) and $\bar{G}^\sigma(i\omega_n)$ in (8), which is equal to $G^{\text{loc}}_\sigma(i\omega_n)$. Below we will not differentiate between $\bar{G}^\sigma(i\omega_n)$ and $G^{\text{loc}}_\sigma(i\omega_n)$ on the understanding that the external fields are determined self-consistently.

A complete solution for the partition functional $Z$ in (3) has not been possible. The exact solution is known for the Falicov-Kimball model [9], for which only one of external fields is needed [23] as only one spin species is allowed to move in this model. In the next section, we derive an approximate solution for the partition functional $Z$ of the $D^\infty$ HM.
3 Approximate partition functional

3.1 Expansion

Since $H_0$ and $V$ commute for the atomic Hamiltonian $H$ in (3), one can write

\[ e^{-\beta H} = e^{-\beta H_0} e^{-\beta V} = e^{-\beta H_0} \sum_{m=0}^{\infty} \frac{(-\beta)^m}{m!} V_m \]

\[ = e^{-\beta H_0} [1 + (e^{-\beta V} - 1)n_{\uparrow} n_{\downarrow}] . \]  

The partition functional of (3) can therefore be expressed

\[ Z = e^{-\beta \Omega_0 \{ \langle S \rangle_0 + (e^{-\beta V} - 1) \langle n_{\uparrow} n_{\downarrow} S \rangle_0 \}}, \]

where $\Omega_0$ is the thermodynamic potential for $H_0$, and $\langle \theta \rangle_0 = \text{Tr}(e^{\beta(\Omega_0-H_0)} \theta)$. The important point to note from (13) is that we need only to calculate expectation values with respect to $H_0$. However, the interaction still appears in the Heisenberg operators $a_{\sigma}^{H\dagger}(\tau)$ and $a_{\sigma}^H(\tau)$ which define $S$ in (7). We represent the operators $a_{\sigma}^{H\dagger}(\tau)$ and $a_{\sigma}^H(\tau)$ in terms of the Heisenberg operators for $H_0$ in a similar way as in (14). We write

\[ a_{\sigma}^{H\dagger}(\tau) = a_{\sigma}^0(\tau) [1 + (e^{U\tau} - 1)n_{-\sigma}(\tau)], \]

\[ a_{\sigma}^H(\tau) = a_{\sigma}(\tau) [1 + (e^{-U\tau} - 1)n_{-\sigma}(\tau)], \]  

where $a_{\sigma}^0(\tau) = e^{H_0 \tau} a_{\sigma} e^{-H_0 \tau}$.

We first look at the expectation value $\langle S \rangle_0$ in (13), which is given by

\[ \langle S \rangle_0 = \langle T_{\tau \theta}[\exp[-\int_0^\beta d\tau \int_0^\beta d\tau' V_{\uparrow}(\tau, \tau')]] \exp[-\int_0^\beta d\theta \int_0^\beta d\theta' V_{\downarrow}(\theta, \theta')]) \rangle_0, \]

where

\[ V_{\sigma}(\tau, \tau') = A_{\sigma}(\tau, \tau') B_{\sigma}(\tau, \tau'), \]

\[ A_{\sigma}(\tau, \tau') = \lambda^e(\tau, \tau') a_{\sigma}^\dagger(\tau) a_{\sigma}(\tau'), \]

\[ B_{\sigma}(\tau, \tau') = [1 + (e^{U\tau} - 1)n_{-\sigma}(\tau)][1 + (e^{-U\tau'} - 1)n_{-\sigma}(\tau')]. \]

Expanding the exponentials in (13) gives

\[ \langle S \rangle_0 = \sum_{mn} \frac{1}{m!n!} \int d\tau \int d\theta X_{mn}(\tau, \theta), \]

where

\[ X_{mn}(\tau, \theta) = \langle T_{\tau \theta}\{ A_{\sigma}^m(\tau) B_{\sigma}^n(\theta) A_{\sigma}^n(\theta) B_{\sigma}^m(\tau) \} \rangle_0, \]

with $A_{\sigma}^m(\tau) = A_{\sigma}(\tau_1, \tau'_1) \ldots A_{\sigma}(\tau_m, \tau'_m)$, and $B_{\sigma}^n(\tau) = B_{\sigma}(\tau_1, \tau'_1) \ldots B_{\sigma}(\tau_m, \tau'_m)$, and the integration in (17) is for all $\tau$’s and $\theta$’s. $A_{\sigma}(\tau)$ and $B_{\sigma}(\tau)$ contain all the operators involving spin-$\sigma$ electrons in (18), and so using Wick’s theorem we can write

\[ X_{mn}(\tau, \theta) = \langle T_{\tau \theta}\{ A_{\sigma}^m(\tau) B_{\sigma}^n(\theta) \} \rangle_0 \langle T_{\tau \theta}\{ A_{\sigma}^n(\theta) B_{\sigma}^m(\tau) \} \rangle_0. \]
The quantity $X_{mn}$ may be calculated for any finite order $m$ and $n$ using Wick’s theorem. However, an analytic calculation up to infinite order including all Feynmann diagrams as required in (17) is not possible. We therefore approximate to find the $X_{mn}$.

### 3.2 Approximation

When evaluating the $X_{mn}$, we will consider only contractions within $\bar{A}_\sigma(\tau)$ and $\bar{B}_{-\sigma}(\theta)$ and ignore those between $\bar{A}_\sigma(\tau)$ and $\bar{B}_{-\sigma}(\theta)$. Note that the effects of the hopping terms in the original Hamiltonian are incorporated via the external fields, $\lambda^\sigma(\tau, \tau')$, included in $\bar{A}_\sigma(\tau)$ [see Eq. (16)]. Roughly speaking, the $\bar{A}_\sigma(\tau)$ account for the “dynamics” of the spin $\sigma$ electrons, while the $\bar{B}_{-\sigma}(\theta)$ monitor the value of $n_\sigma$ at the times, $\theta$, at which $-\sigma$ occupation changes. Restricting contractions to within $\bar{B}_{-\sigma}(\theta)$ sets up a mean ‘$-\sigma$’ field for the motion of the $\sigma$ electrons and vice versa. As we will see, $\langle T_\theta \bar{B}_{-\sigma}(\theta) \rangle$ gives rise to two terms which describe propagation in the upper and lower Hubbard bands.

Our approximation is in the spirit of the Gutzwiller approximation for Gutzwiller wave function [24]. Gutzwiller’s original idea was to treat the down-spin electrons as static when considering the motion of the up-spin eletron, and vice versa. This approximation does not break the spin-symmetry and keeps the translational invariance, so that Fermi-liquid behavior can exist at zero temperature. The ground state energy per site for the Hubbard model like Eq. (1) can be written as

$$E = \frac{1}{N} \sum_{k,\sigma} q_\sigma \epsilon_k n_{k\sigma} + Ud,$$

where $n_{k\sigma}$ is the fermion distribution function and $d$ is the double occupancy per site. The effects of one spin species on the other are incorporated into the renormalization factor, $q_\sigma$. Eq. (20) has been rederived statistically [25] and the Gutzwiller approximation has been shown to be exact in the limit of infinite dimensions [2].

Only considering the contractions within $\bar{A}_\sigma(\tau)$ and $\bar{B}_{-\sigma}(\theta)$ is equivalent to decoupling $\bar{A}_\sigma(\tau)$ and $\bar{B}_{-\sigma}(\theta)$. Writing $\langle T_\tau \bar{A}_\sigma^m(\tau) \rangle_0 \langle T_\theta \bar{B}_{-\sigma}^n(\theta) \rangle_0$ gives

$$\langle T_\theta \bar{B}_{-\sigma}^n(\theta) \rangle_0 = \langle [1-n_\sigma] + \exp\{U \sum_{i=1}^n (\theta_i - \theta_i') \} n_\sigma \rangle_0. \quad (21)$$

Accounting for the first term of (21), when multiplied by $\langle T_\tau \bar{A}_\sigma^m(\tau) \rangle_0$, is straightforward. Summing over $m$ for $\langle T_\tau \bar{A}_\sigma^m(\tau) \rangle_0$ yields

$$\langle S_\sigma \rangle_0 = \sum_{m=0}^{\infty} \frac{1}{m!} \langle T_\tau \bar{A}_\sigma^m(\tau) \rangle_0$$

$$= \langle T_\tau \exp\{- \int_0^\beta d\tau' \int_0^\beta d\tau' \lambda^\sigma(\tau, \tau') a_\sigma(\tau') a_\sigma(\tau) \} \rangle_0$$

$$= \exp\{\sum_{n} \ln[1-n_\sigma g_\sigma^0(i\omega_n)]\},$$

with

$$g_\sigma^0(i\omega_n) = \frac{1}{i\omega_n - (E_\sigma - \mu)}. \quad (23)$$
The second term provides a time-dependent “potential” [the exponential in \((24)\)] which affects the dynamics of \(\tilde{A}_{\uparrow,\sigma}^{m}(\theta)\) of the \(-\sigma\) electrons. This term essentially changes the external field \(\lambda_{\uparrow,-\sigma}(\theta,\theta')\) to \(\lambda_{\uparrow,-\sigma}(\theta,\theta')\exp{\{U(\theta - \theta')\}}\). Summing over \(n\) for \(\tilde{A}_{\uparrow,\sigma}^{n}(\theta)\), one needs to calculate an expectation value of the type

\[
\langle \tilde{S}_{\uparrow,\sigma} \rangle_{0} = \exp{-\int_{0}^{\beta} d\theta \int_{0}^{\beta} d\theta' \lambda_{\uparrow,-\sigma}(\theta,\theta') e^{U(\theta - \theta')} a_{\uparrow,-\sigma}^{\dagger}(\theta) a_{\uparrow,-\sigma}(\theta')}_{0}.
\]

These can not be dealt with as in \((22)\) because of the non-periodicity of \(\lambda_{\uparrow,-\sigma}(\theta,\theta')\). However, introducing the Hamiltonian

\[
\tilde{H}_{\uparrow,-\sigma} = H_{0} + U a_{\uparrow,-\sigma}^{\dagger} a_{\uparrow,-\sigma},
\]

and defining new Heisenberg operators with respect to \(\tilde{H}_{\uparrow,-\sigma}\): 
\(\tilde{a}_{\uparrow,-\sigma}^{\dagger}(\theta) = e^{U\theta} a_{\uparrow,-\sigma}^{\dagger}(\theta)\), we can easily calculate the expectation value

\[
\langle \tilde{S}_{\uparrow,\sigma} \rangle_{\tilde{H}_{\uparrow,-\sigma}} = \exp{-\int_{0}^{\beta} d\theta \int_{0}^{\beta} d\theta' \lambda_{\uparrow,-\sigma}(\theta,\theta') \tilde{a}_{\uparrow,-\sigma}^{\dagger}(\theta) \tilde{a}_{\uparrow,-\sigma}(\theta')}_{\tilde{H}_{\uparrow,-\sigma}},
\]

\[
= \exp{\sum_{n} \ln(1 - \lambda_{n}\tilde{g}_{\uparrow,-\sigma}(i\omega_{n}))}.
\]

Here

\[
\tilde{g}_{\uparrow,-\sigma}(i\omega_{n}) = \frac{1}{i\omega_{n} - (E_{\uparrow,-\sigma} - \mu - U)}.
\]

and \(\langle \theta \rangle_{\tilde{H}_{\uparrow,-\sigma}} = Tr e^{\beta(\tilde{H}_{\uparrow,-\sigma} - H_{\uparrow,-\sigma})} \theta\). It is clear that \((25)\) describes motion of electrons in the upper Hubbard band, while \((22)\) comes from motion in the lower Hubbard band. This is reminiscent of the alloy analogy approximation (AAA), where the lower and upper Hubbard bands are introduced explicitly. However, as we shall see, our approximation avoids the most serious fault of the AAA and does not violate the Luttinger theorems at \(T = 0\), which allows the metallic behavior.

The expectation values of the operators \(\tilde{B}_{\uparrow,\sigma}^{m}(\theta)\) always lead to a contribution proportional to \(\langle (1 - n_{\uparrow}) \rangle\) and a time-dependent term \(\langle \exp{\{U \sum_{i=1}^{m}(\theta_{i} - \theta_{i}')\} n_{\uparrow} \}}\). We then incorporate the exponential in the latter term directly into an operator \(\tilde{A}_{\uparrow,-\sigma}^{m}(\theta) = e^{U\theta} A_{\uparrow,-\sigma}^{m}(\theta) \exp{\{U \sum_{i=1}^{m}(\theta_{i} - \theta_{i}')\}}\). Our decoupling procedure for this term is equivalent to writing for any function \(F[n_{\uparrow,\sigma}(\theta)]\)

\[
T_{\theta}\{e^{\beta(\Omega_{0} - H_{0})} \tilde{A}_{\uparrow,-\sigma}^{m}(\theta) e^{\beta(U n_{\uparrow,\sigma} - F[n_{\uparrow,\sigma}(\theta)])} \}
\]

\[
\approx \langle T_{\theta}\tilde{A}_{\uparrow,-\sigma}^{m}(\theta) \rangle_{\tilde{H}_{\uparrow,-\sigma}} \{e^{\beta(U n_{\uparrow,\sigma} - F[n_{\uparrow,\sigma}(\theta)])} \}
\]

We can see that the upper Hubbard band is introduced naturally at the decoupling stage. This procedure must be carried out for \(\tilde{B}_{\uparrow,\sigma}^{m}(\tau)\) as well.

The final result for the decoupling of the \(X_{mn}(\tau,\theta)\) in \((19)\) is

\[
X_{mn}(\tau,\theta) \approx \langle T_{\tau} \tilde{A}_{\uparrow}^{m}(\tau) \rangle_{0} (1 - n_{\uparrow})_{0} \langle T_{\theta} \tilde{A}_{\uparrow}^{n}(\theta) \rangle_{0} (1 - n_{\downarrow})_{0}
\]

\[
+ \langle T_{\tau} \tilde{A}_{\uparrow}^{m}(\tau) \rangle_{H_{\uparrow}} \{e^{\beta U n_{\uparrow}(1 - n_{\uparrow})} \} \langle T_{\theta} \tilde{A}_{\uparrow}^{n}(\theta) \rangle_{H_{\downarrow}} e^{\beta(\Omega_{0} - H_{0})} \langle(T_{\theta} \tilde{A}_{\uparrow}^{n}(\theta))_{0} (n_{\downarrow})_{0}
\]

\[
+ \langle T_{\tau} \tilde{A}_{\uparrow}^{m}(\tau) \rangle_{0} (n_{\uparrow})_{0} \langle T_{\theta} \tilde{A}_{\uparrow}^{n}(\theta) \rangle_{\tilde{H}_{\uparrow}} \{e^{\beta U n_{\uparrow}(1 - n_{\uparrow})} \} \langle(T_{\theta} \tilde{A}_{\uparrow}^{n}(\theta))_{\tilde{H}_{\uparrow}} e^{\beta(\Omega_{0} - H_{0})}
\]

\[
+ \langle T_{\tau} \tilde{A}_{\uparrow}^{m}(\tau) \rangle_{\tilde{H}_{\uparrow}} \{e^{\beta U n_{\uparrow}(1 - n_{\uparrow})} \} \langle T_{\theta} \tilde{A}_{\uparrow}^{n}(\theta) \rangle_{\tilde{H}_{\downarrow}} \{e^{\beta U n_{\uparrow}(1 - n_{\uparrow})} \} \langle T_{\theta} \tilde{A}_{\uparrow}^{n}(\theta) \rangle_{\tilde{H}_{\downarrow}} e^{\beta \sum_{\sigma}(\Omega_{0} - H_{0}).(28)\}
\]
where $\Omega_{\sigma}$ is the thermodynamic potential of $\tilde{H}_\sigma$. Eq. (28) is the main approximation we make for the partition functional.

This approximation leads us to a form for $\langle S \rangle_0$

\[
\langle S \rangle_0 = \langle S \rangle_0[1 - \langle n_\uparrow \rangle_0]\langle S \rangle_0[1 - \langle n_\downarrow \rangle_0]
+ \langle S \rangle_0[1 - \langle n_\uparrow \rangle_\tilde{H}_\uparrow]\langle S \rangle_0[n_\downarrow]e^{\beta(\Omega_0 - \Omega)}
+ \langle S \rangle_0[n_\uparrow]\langle S \rangle_0[1 - \langle n_\downarrow \rangle_\tilde{H}_\downarrow]e^{\beta(\Omega_0 - \Omega)}
+ \langle S \rangle_0[\bar{n}_\sigma]e^{\beta U}[\bar{n}_\sigma]e^{\beta U}[\bar{n}_\sigma]e^{\beta \sum_\sigma(\Omega_0 - \Omega_\sigma)},
\]

where $\langle S \rangle_0$ and $\langle S \rangle_0$ are given by (23) and (25), respectively. The expectation value of the term $\langle n_\uparrow n_\downarrow S \rangle_0$ in (13) is then given by

\[
\langle n_\uparrow n_\downarrow S \rangle_0 = \langle S \rangle_0[1 + \langle n_\uparrow \rangle_\tilde{H}_\uparrow]\langle S \rangle_0[n_\downarrow]e^{\beta U}[n_\downarrow]e^{\beta \sum_\sigma(\Omega_0 - \Omega_\sigma)}.
\]

Using (13), (29) and (30), we obtain the partition functional

\[
Z = \begin{pmatrix} \bar{Z}_\uparrow & \bar{Z}_\downarrow \end{pmatrix} \begin{pmatrix} (1 - \bar{n}_\uparrow)(1 - \bar{n}_\downarrow) & \bar{n}_\uparrow(1 - \bar{n}_\downarrow) \\ (1 - \bar{n}_\uparrow)\bar{n}_\downarrow & \bar{n}_\uparrow \end{pmatrix} \begin{pmatrix} \bar{Z}_\uparrow \\ \bar{Z}_\downarrow \end{pmatrix}.
\]

Here

\[
\bar{Z}_\sigma = \exp\{\sum_n \ln[i\omega_n - (E_\sigma - \mu) - \lambda_n]\},
\]

\[
\bar{Z}_\sigma = \exp\{\sum_n \ln[i\omega_n - (E_\sigma - \mu) - U - \lambda_n]\},
\]

\[
\bar{n}_\sigma \equiv \langle n_\sigma \rangle_0 = [e^{\beta(E_\sigma - \mu)} + 1]^{-1},
\]

\[
\bar{n}_\sigma \equiv \langle n_\sigma \rangle_\tilde{H}_\sigma = [e^{\beta(E_\sigma - \mu + U)} + 1]^{-1}.
\]

The partition functional $Z$ in (31) has a very natural interpretation. $\bar{n}_\sigma$ and $\bar{Z}_\sigma$ can be regarded, respectively, as the “occupancy” and the “partition function” of the spin $\sigma$ particles in the lower Hubbard band, while $\bar{n}_\sigma$ and $\bar{Z}_\sigma$ are the corresponding quantities in the upper Hubbard band. The terms with $(1 - \bar{n}_\uparrow)(1 - \bar{n}_\downarrow)$, $\bar{n}_\uparrow(1 - \bar{n}_\downarrow)$, or $(1 - \bar{n}_\uparrow)\bar{n}_\downarrow$ and $e^{\beta U}\bar{n}_\uparrow\bar{n}_\downarrow$ in the matrix account for holes, singly-occupied and doubly-occupied configurations, respectively. The factor $e^{\beta U}$ is essential because it cancels the double counting of the interaction $U$ involved in $\bar{Z}_\uparrow\bar{Z}_\downarrow$. Comparing the form of the ground state energy $E$ of the Gutzwiller approximation in (20) with $Z$ in (31), we see that the “configuration” matrix in $Z$ gives a function like the renormalized constant $q_\sigma$ in $E$.

For the $D^\infty$ Falicov-Kimball model, where one of the external fields, $\lambda^\uparrow$ say, equals zero, Eq. (31) reduces to

\[
Z_{FK} = \bar{Z}_\uparrow + \bar{Z}_\downarrow e^{\beta(U - \mu)},
\]

which is just the result obtained by Brandt and Mielsch [9]. Therefore, our partition functional naturally includes the exact solution of the Falicov-Kimball model as a special case. It is also easy to check that (31) gives the exact result for the atomic ($t = 0$) and $U = 0$ limits.
4 Thermodynamic properties

4.1 The Green’s function and physical quantities

Using (31) and (10), one can obtain the self-energy functional. Substituting this functional into the right hand side of the self-consistent equation in (3), and noting from (9) that the left hand side can be written

\[ G_{\text{loc}}^{\sigma}(\omega_n) = \left[ i\omega_n - (E_\sigma - \mu) - \lambda_\sigma n - \Sigma_\sigma(\omega_n) \right]^{-1}, \]  

one can determine the external fields self-consistently. Consequently, the self-energy and the Green’s function for the \( D_\infty \) HM are easily found using this approximation.

If the external fields are fixed, it is convenient to use another form of the local Green’s function derived directly from the functional derivative in (9),

\[ G_{\text{loc}}^{\sigma}(\omega_n) = \bar{G}_\sigma(\omega_n)P_0 + \tilde{G}_\sigma(\omega_n)P_1, \]  

where

\[ \bar{G}_\sigma(\omega_n) = \left[ i\omega_n - (E_\sigma - \mu) - \lambda_\sigma \right]^{-1}, \]
\[ \tilde{G}_\sigma(\omega_n) = \left[ i\omega_n - (E_\sigma - \mu) - U - \lambda_\sigma \right]^{-1}, \]  

and

\[ P_0 = \frac{1}{Z}[Z_\uparrow(1 - \bar{n}_\uparrow)(1 - \tilde{n}_\downarrow)\bar{Z}_\downarrow + Z_\downarrow\bar{n}_\uparrow(1 - \tilde{n}_\downarrow)\bar{Z}_\uparrow], \]
\[ P_1 = \frac{1}{Z}[\bar{Z}_\uparrow(1 - \tilde{n}_\uparrow)\bar{n}_\downarrow\tilde{Z}_\downarrow + \tilde{Z}_\downarrow e^{\beta U} \bar{n}_\uparrow\tilde{n}_\downarrow\tilde{Z}_\uparrow]. \]

Clearly, \( P_0 + P_1 = 1 \). Again, the Green’s function \( G_{\text{loc}}^{\sigma}(\omega_n) \) looks similar to that given by the alloy analogy approximation [12]. However, \( P_0 \) and \( P_1 \) have quite different forms. We will see later that this difference leads to important consequences.

Using (33), the density states of the system can be expressed as

\[ D_\sigma(\omega_n) = \bar{D}_\sigma(\omega_n)P_0 + \tilde{D}_\sigma(\omega_n)P_1, \]  

where

\[ \bar{D}_\sigma(i\omega) = -\frac{1}{2\pi i}[\bar{G}_\sigma(\omega + i0^+) - \tilde{G}_\sigma(\omega - i0^+)], \]
\[ \tilde{D}_\sigma(i\omega_n) = -\frac{1}{2\pi i}[\bar{G}_\sigma(\omega + i0^+) - \tilde{G}_\sigma(\omega - i0^+)]. \]  

The chemical potential should be determined self-consistently from the following equation for the electron concentration

\[ n_\sigma(T) = \int_{-\infty}^{\infty} d\epsilon f(\epsilon)D_\sigma(\epsilon), \]  

where \( f(\epsilon) \) is the fermion distribution function and \( D_\sigma(\epsilon) \) is given in (38).
From the Green’s function (35), one can calculate all thermodynamic quantities of the systems. In this paper we discuss the susceptibility, specific heat and resistivity of the system.

The static susceptibility can be obtained directly by differentiating the occupancy, $n_\sigma$, in (40) with respect to $E_\sigma$. We set $E_\sigma = -\sigma \mu_B h$, with $h$ the external magnetic field. The susceptibility, $\chi(T)$, is then

$$\chi(T) = \left. \frac{\partial [\mu_B (n_\uparrow - n_\downarrow)]}{\partial h} \right|_{h=0} = -2 \mu_B^2 \left( \left. \frac{\partial n_\uparrow}{\partial E_\uparrow} - \frac{\partial n_\downarrow}{\partial E_\downarrow} \right|_{E_\uparrow = E_\downarrow = 0} \right) \quad (41)$$

In order to obtain the specific heat, it is convenient (especially for numerical calculations) to start from the internal energy, $E(T)$. This enables us to calculate the specific heat $C(T)$ as the first derivative of $E(T)$ with respect to $T$ rather than the second derivative of the free energy. In the infinite-dimensional case, $E(T)$ is given by

$$E(T) = -\sum_\sigma \int d\epsilon \rho_0(\epsilon) \int \frac{d\omega}{2\pi} f(\epsilon + \omega) \text{Im} \frac{1}{\omega + \mu - \Sigma_r(\omega) - \epsilon + i\delta} + \frac{1}{2} \mu n, \quad (42)$$

where $\rho_0(\epsilon)$ is the bare density of states.

The conductivity is expressed using Kubo’s formula as a current-current correlation function. Usually this correlation function can not be calculated exactly since the vertex corrections are difficult to treat. However, in the infinite $D$ limit, vertex corrections vanish \[27\], so that one is left with a simple bubble for the conductivity correlation function. The conductivity becomes

$$\sigma(0) = 2 \int_{-\infty}^{\infty} d\epsilon \rho_0(\epsilon) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (-\frac{\partial f(\omega)}{\partial \omega}) A(\epsilon, \omega)^2, \quad (43)$$

where the spectral function $A(\epsilon, \omega)$ is defined as

$$A(\epsilon, \omega) = i[G_r(\epsilon, \omega) - G_a(\epsilon, \omega)]$$

$$= i \left[ \frac{1}{\omega + \mu - \Sigma_r + i\eta - \epsilon} - \frac{1}{\omega + \mu - \Sigma_a - i\eta - \epsilon} \right], \quad (44)$$

with $\Sigma_r$ and $\Sigma_a$ the retarded and advanced self-energy of the system, respectively. We have set $\hbar = e = a = 1$ ($a$ is the lattice constant) in (43).

### 4.2 The Lorentzian bare density of states

To illustrate the scheme we use a Lorentzian type for the bare DOS \[10, 19\]:

$$\rho_0(\epsilon) = \frac{\Gamma}{\pi} (\epsilon^2 + \Gamma^2). \quad (45)$$

Although this DOS has some undesirable properties as a result of having too much weight at large energies, it leads to some analytical results and some analytical expressions for physical quantities. Apart from the Mott transition, the physical properties are expected to be qualitatively correct for this DOS \[19\].
For the Lorentzian DOS, Eq. (3) reduces to

\[ G_{\sigma}^{\text{loc}}(i\omega_n) = [i\omega - (E_{\sigma} - \mu) - \Sigma_{\sigma}(i\omega_n) + i\Gamma \text{sgn}\omega_n ]^{-1}. \] (46)

Comparing this with Eq. (34), one immediately obtains the external field

\[ \lambda_n = -i\Gamma \text{sgn}\omega_n. \] (47)

Substituting (47) into (35) and (10) gives the Green’s function \( G_{\sigma}^{\text{loc}}(i\omega_n) \) and the self-energy \( \Sigma(i\omega_n) \) for a system with a Lorentzian DOS. A frequency summation then gives \( \bar{Z}_{\sigma} \) and \( \tilde{Z}_{\sigma} \) in (31)

\[ \bar{Z}_{\sigma} = C e^{\beta u_{\sigma}(E_{\sigma} - \mu)}, \]
\[ \tilde{Z}_{\sigma} = C e^{\beta u_{\sigma}(E_{\sigma} + U - \mu)}, \] (48)

where \( C \) is a constant, which is irrelevant for the thermodynamic properties, and the function

\[ u_{\sigma}(x) = \int_{0}^{-x} d\lambda \int_{-\infty}^{\infty} f(z - \lambda) \rho_0(z) dz. \] (49)

At zero temperature, \( \bar{Z}_{\sigma} \) in (48) reduces

\[ Z_{\sigma} = C \exp\{\beta\{\frac{\mu - E_{\sigma}}{2} + \frac{1}{\pi}[\mu - E_{\sigma} - U]\arctan\frac{\mu - E_{\sigma}}{\Gamma} - \frac{\Gamma}{2}\ln(1 + \frac{\mu - E_{\sigma}}{\Gamma^2})]\}\}, \] (50)

while \( \tilde{Z}_{\sigma} \) has the same form as \( \bar{Z}_{\sigma} \) but with \( E_{\sigma} \) replaced by \( E_{\sigma} + U \).

We find that for the electron concentration \( n (= n_\uparrow + n_\downarrow) \) less than one, the term with \( (1 - \bar{n}_\uparrow)(1 - \bar{n}_\downarrow) \) in \( Z \) of (31) is dominant, and \( P_1 \) vanishes. The chemical potential can easily be obtained from (40)

\[ \mu = -\Gamma \tan\frac{\pi}{2}(1 - n) \quad \text{(for } n < 1). \] (51)

For \( n > 1 \), the term with \( e^{\beta U \bar{n}_\uparrow \bar{n}_\downarrow} \) in \( Z \) is dominant (so that \( P_1 = 1 \)) and the chemical potential is given by

\[ \mu = U + \Gamma \tan\frac{\pi}{2}(n - 1) \quad \text{(for } n > 1). \] (52)

For \( n = 1 \), the terms with \( \bar{n}_\uparrow(1 - \bar{n}_\downarrow) \) [and \( (1 - \bar{n}_\uparrow)\bar{n}_\downarrow \)] in \( Z \) are important and the chemical potential \( \mu = U/2 \), as it should be. The chemical potential \( \mu \) is shown in Fig. 1 as a function of the electron concentration \( n \).

From (40) we find that the imaginary part of the self-energy at \( \omega = 0 \) is equal to zero away from half-filling and the Luttinger theorem is satisfied. The system is in a Fermi-liquid state. This is consistent with the exact statement of Georges and Kotliar [1]. However, at half-filling the imaginary part of the self-energy at \( \omega = 0 \) is not equal to zero and there is a discontinuity at the chemical potential, as shown in Fig. 1. At half-filling the system is therefore a Mott insulator for any finite \( U \). This is similar to what happens in the one-dimensional case [1], but is inconsistent with Monte Carlo calculations [3], which show that the Mott insulating state appears for all \( U \geq 3 \).
occurrence of a Mott insulating state at half-filling follows in our approximation as a result of the particle-hole symmetry and is not an artefact of using the Lorentzian density of states. The absence of a Mott transition at finite \( U \) in our approximation results from overcounting of the interaction effect for small \( U \), i.e. for the same reason as given by Hubbard for his Hubbard-II approximation \[28\].

The susceptibility is given by

\[
\chi = 2\mu_B^2 \left[ \frac{P_0}{\pi} \frac{\Gamma}{\mu^2 + \Gamma^2} + \frac{P_0}{\pi} \frac{\Gamma}{(\mu - U)^2 + \Gamma^2} \right],
\]

which has no divergence for any \( n \) and finite \( U \), so that there is no ferromagnetic phase.

The temperature dependence of the static susceptibility \( \chi \) and the specific heat \( C \) are shown in Fig.2. (The temperature \( T \) and the interaction \( U \) are in units of \( \Gamma \).) At high temperature, \( \chi \) shows a Curie-Weiss-like behavior (\( \chi \sim 1/(T + \theta) \) with \( \theta > 0 \)), indicating that the system behaves like a system of independent moments with antiferromagnetic fluctuations. For \( n \) near half-filling or for large \( U \), \( \chi \) decreases as \( T \) drops below a characteristic temperature, \( T^* \), in a way reminiscent of the Kondo effect (see curves A and B). Near \( T^* \), the specific heat also has a peak. For the susceptibility there appears to be a second temperature \( T_1^* \), below which a correlated state is formed where the susceptibility is nearly constant, i.e., Pauli-like. At \( T_1^* \) there is no anomaly in the specific heat. For small \( n \), the susceptibility continuously crosses over from the Curie-Weiss behavior to the Pauli-like behavior without any Kondo-like anomaly. Correspondingly the specific heat shows no peak. At very low temperature, the specific heat as a function of \( T \) is consistent with a power law, but with an exponent not exactly equal to one, i.e. the behavior is not exactly linear. The case of the Lorentzian density of states corresponds to the Anderson impurity model \[10\] with \( \epsilon_d = \mu(T) \), where \( \epsilon_d \) is the d-level energy. The impurity model has been solved exactly for fixed \( \epsilon_d \) and does give \( C_v \propto T \). However, in our case the chemical potential \( \mu \) is a function of temperature, which must be determined self-consistently. This has not yet been done. The variation of \( \mu \) with \( T \) will change the impurity model result for \( C_v \). It is therefore not clear whether our result is actually correct or a result of the approximation.

In order to understand the “Kondo anomaly” in this system, we calculate the density of states, shown in Fig. 3 for the case of \( U = 2 \) and \( n = 0.8 \). There are two peaks above a certain temperature, which corresponds to the “Kondo” characteristic temperature \( T^* \). There is only one peak below this temperature. The Kondo anomaly seems to be related to the appearance of the Hubbard pseudo-gap. The self-consistent perturbation calculations also show one peak in the DOS of the system at zero temperature \[21, 29\]. However, using the perturbation scheme of Yosida and Yomada \[30\], Georges and Kotliar \[10\] found that the DOS has two peaks near half-filling at zero temperature. The one-peak feature found at very low temperature obtained using the self-consistent perturbation calculation might indicate that the upper band does not contribute much to thermodynamic properties at low temperature and the Hubbard pseudo-gap behavior manifests itself only above a characteristic temperature.

The temperature dependence of the resistivity \( \rho (= 1/\sigma) \) is shown in Fig. 4 (for \( U = 2 \)) and Fig. 5 (for \( U = 4 \)) for various electron concentrations. The resistivity goes to zero when temperature decreases to zero as it should, given that our approximation satisfies
the Luttinger theorem at zero temperature. This is in contrast with the result of the alloy analogy approximation (shown schematically by the dashed curve in Fig. 4), which keeps rising as temperature decreases. The resistivity becomes roughly linear with \( T \) above the characteristic temperature, while it rises rapidly around the characteristic temperature. In order to see clearly how fast \( \rho \) changes with \( T \), we show in Fig. 6 the first derivative of \( \rho \) with respective to \( T \) in the case of \( U = 2 \). There is a sharp peak at the characteristic temperature.

5 Discussion and conclusion

In this paper we have derived an approximate self-energy functional for the infinite-dimensional Hubbard model. It naturally includes the exact solution of the \( D^\infty \) Falicov-Kimball model as a special case and retains the spin symmetry. This finite-temperature theory successfully incorporates the high-temperature uncorrelated behavior and the strongly correlated behavior at low temperature in a unified way. Many approximations used before, such as the alloy analogy approximation, the equation-of-motion decoupling, the extension of the Gutzwiller approach and the slave boson mean-field theory, cannot reproduce both limiting behaviors correctly without introducing a spurious phase transition \([16] [12]\). It seems to us that our approach is the first to give physically reasonable results for all temperatures.

The functional derived here is very easy to use. It can also be directly applied to the periodic Anderson model. The only change is to replace the self-consistent equation in (3) by

\[
G_{f\sigma}^{\text{loc}} = \int_{-\infty}^{\infty} \frac{\rho_0(\epsilon)d\epsilon}{i\omega_n - (\epsilon - \mu) - \Sigma_{f\sigma}(i\omega_n) - V^2/i\omega_n - (\epsilon - \mu)},
\]

where “\( f \)” represents localized electrons, and \( V \) is the mixing energy between conduction and localized electrons. From (54) one can determine the local Green’s function and the self-energy of the localized electrons, and consequently, all Green’s functions of the system \([31]\).

In this paper we have treated only the case of a homogeneous system. For some symmetry-broken phases, such as the antiferromagnetic state, the self-consistent equation changes \([34]\), although the form of self-energy functional remains. Because our scheme treats spin-up and spin-down electrons on an equal footing (in contrast to the alloy analogy approximation), we expect that it can describe correctly the antiferromagnetic instability. We will discuss this issue elsewhere \([32]\).

There exist some weaknesses in the present form of the partition function. The dynamic fluctuations induced by the motion of one spin species to another are not properly treated. Moreover, the Mott transition does not take place at a finite interaction \( U \). Since our approximation is an expansion, we can include relevant higher order contributions which account for these fluctuations. The Mott transition has been produced by Hubbard in his Hubbard-III paper \([15]\) by including the resonant correction in the equivalent coherent-potential approximation. It would be interesting to examine this transition in our formalism by including higher order fluctuation effects since our solu-
tion satisfies the Luttinger theorem in the metallic side at zero temperature, while the Hubbard-III solution does not [33].

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FIGURE CAPTIONS

Fig.1. The chemical potential \( \mu \) as a function of the electron concentration \( n \) at zero temperature. \( \mu \) is in unit of \( \Gamma \). The gap at half-filling is present for all non-zero \( U \).

Fig.2. The temperature dependence of the susceptibility, \( \chi \) (solid curve), and the specific heat \( C \) (dashed curve) for the Lorentzian density of states for various \( n \) and \( U \). Curves \( A \) & \( a \) are for \( U = 1 \) and \( n = 0.9 \), while \( B \) & \( b \), \( C \) & \( c \) and \( D \) & \( d \) correspond to \( n = 0.8, 0.6 \) and \( 0.4 \), respectively, for the case of \( U = 2 \). \( T \) and \( U \) are in units of \( \Gamma \), and \( \chi \) is in unit of \( \mu_B^2 \).

Fig.3. The density of states of the system, \( D(\omega) \), for various temperatures in the case of \( U = 2 \) and \( n = 0.8 \).

Fig.4. The temperature dependence of the resistivity for \( U = 2 \) and various electron concentration \( n \). The result of the alloy analogy approximation is schematically shown by the dashed curve.

Fig.5. The temperature dependence of the resistivity for \( U = 4 \) and various \( n \).

Fig.6. The first derivative of the resistivity with respect to temperature for \( U = 2 \), corresponding to Fig. 4.