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Mixtures of fermionic atoms in an optical lattice

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A mixture of light and heavy spin-polarized fermionic atoms in an optical lattice is considered. Tunneling of the heavy atoms is neglected such that they are only subject to thermal fluctuations. This results in a complex interplay between light and heavy atoms caused by quantum tunneling of the light atoms. The distribution of the heavy atoms is studied. It can be described by an Ising-like distribution with a first-order transition from homogeneous to staggered order. The latter is caused by an effective nonlocal interaction due to quantum tunneling of light atoms. A second-order transition is also possible between an ordered and a disordered phase of heavy atoms.

1. INTRODUCTION: PHASE SEPARATION AND THE PHYSICS OF CORRELATED DISORDER

Mixtures of different species of cold atoms open an interesting field of many-body physics, where the competition between the atoms may lead to new quantum states. This is the case for low-temperature properties (i.e. for the ground state) as well as in the presence of thermal fluctuations. For the latter case we expect phase separation, where different phases can coexist. This phenomenon has been intensively discussed in the solid-state community in the context of complex materials [1], and it is believed to be a result of the competition of different (e.g. spin and orbital) degrees of freedom [2]. A similar situation may appear in atomic mixtures due to correlations caused by the competition of the different atomic species. Two or more phases can coexist if there is a first-order phase transition between the individual phases. In other words, thermal fluctuations lead to metastable states that decay only on long-time scales. Such a phenomenon is characterized by a broken translational invariance. In terms of an atomic mixture in an optical lattice the atoms are arranged in clusters, consisting of one of the phases, with a characteristic length scale relative to the optical lattice constant. This implies a specific type of correlated disorder that has interesting dynamical properties of the mixtures, including the localization of atoms.

The physics of disorder in statistical or solid-state physics is associated with random scattering of light particles by a *disordered* (i.e. a randomly produced) array of slow particles. This disordered array is static and does not change during the course of the considered scattering process. For instance, the scattering of electrons in a crystal with randomly distributed impurity atoms is a typical realization of disordered physics or the scattering of photons in atmospheric dust.

A comparable situation is found in an atomic system subject to an optical lattice. The periodic structure of the optical lattice, given by counterpropagating lasers, is normally

quite robust such that disorder in the sense of impurities cannot easily be achieved. However, in contrast to a crystal in solid-state physics, two or more different types of atoms can be mixed and brought in an optical lattice, where one type of the atoms is relatively light (e.g. ${}^6\text{Li}$) and the other type(s) is (are) heavy (e.g. ${}^{40}\text{K}$, ${}^{23}\text{Na}$ [3], ${}^{87}\text{Rb}$). The different masses lead to different dynamical properties. In particular, heavy atoms behave almost like static degrees of freedom, in comparison to the light atoms. Therefore, heavy atoms play the role of the impurity atoms in the crystal and the light atoms the role of the electrons. Thus disorder physics can be studied in mixtures of atoms with different masses which are available in experiments [4]. The main difference is here that we shall study the interaction of two species of atoms within the same model. In other words, the distribution of disorder (i.e. the distribution of the heavy atoms) is a direct consequence of the interaction between light and heavy atoms.

Disordered systems have attracted a lot of attention because they provide a new class of physics, including new phases and new types of phase transitions. The main reason is that scattering of quantum particles by a periodic structure is qualitatively different from scattering by a disordered structure: The former is governed by Bloch's Theorem [5] which states that the scattered quantum states are not strongly affected by the scattering process but keep their wave-like properties like the unscattered states. This changes dramatically as soon as the periodicity of the scatterers is disturbed. At first the quantum states lose their wave-like character because the physics is controlled by diffusion. And for stronger disorder the quantum states can even be localized [6]. There is a phase transition between the diffusion-controlled regime and the localized regime [7].

A fundamental concept for a theoretical description of disordered system is that physical quantities are averaged with respect to a statistical distribution of the random structures. It will be discussed in this article that averaging over thermal fluctuations of heavy atoms provides such a type of disorder (or quenched) average of physical quantities, like the density or the dynamical Green's function of a light atom. Emphasis is on fermionic systems, since the appearance of Bose-Einstein condensation should not be included in the discussions. Moreover, there is a formal mapping of the heavy fermions to Ising spins (correlated binary alloy). This provides the opportunity to discuss the statistics in terms of para-, ferro- and antiferromagnetic Ising states.

The article is organized as follows: In Sect. 2 the model of a mixture of two types of atoms is discussed for light and heavy fermionic atoms. The effective distribution of the heavy atoms is studied in Sect. 3, where it is shown that for fermionic atoms this distribution is related to a classical Ising-spin model. The distribution of the Ising spins is investigated in Sect. 3.1, using a strong-coupling expansion.

2. MODEL

A mixture of two types of atoms is considered. The atoms are subject to thermal fluctuations that are treated within a grand-canonical ensemble. Moreover, it is assumed that the atoms are in a magnetic trap such that they are spin polarized. There is a local repulsive interaction between the two species but no other interaction of the atoms within the same species.

c^\dagger (c) are creation (annihilation) operators of the light fermionic atoms, f^\dagger (f) are the

corresponding operators of the heavy fermionic atoms. This gives the formal mapping ${}^6\text{Li} \longrightarrow c_r^\dagger, c_r$ and ${}^{40}\text{K} \longrightarrow f_r^\dagger, f_r$. The physics of the mixture of atoms is defined by the (asymmetric Hubbard) Hamiltonian:

$$H = -\bar{t}_c \sum_{\langle r, r' \rangle} c_r^\dagger c_{r'} - \bar{t}_f \sum_{\langle r, r' \rangle} f_r^\dagger f_{r'} + \sum_r \left[-\mu_c c_r^\dagger c_r - \mu_f f_r^\dagger f_r + U f_r^\dagger f_r c_r^\dagger c_r \right]. \quad (1)$$

An effective interaction among fermionic species is controlled by the (repulsive) Pauli principle.

The tunneling rate decreases exponentially with the square root of the mass of the particle. If the f atoms are heavy, the related tunneling rate is approximated by $\bar{t}_f \approx 0$. This model is known as the Falicov-Kimball model [8–10].

A grand-canonical ensemble of atoms in an optical lattice is a situation in which the optical lattice can exchange atoms with a surrounding atomic cloud. This case is described at the temperature $1/\beta$ by the partition function Z and by the real-time Green's function of light atoms $G_c(r, it; r', 0)$:

$$Z = \text{Tr} e^{-\beta H}, \quad G_c(r, it; r', 0) = \frac{1}{Z} \text{Tr} \left[e^{-\beta H} c_r e^{itH} c_{r'}^\dagger e^{-itH} \right].$$

The density of heavy atoms $n_{f,r}$ and of light atoms $n_{c,r}$ can be obtained from the Green's function in the special case $t = 0, r' = r$.

3. ISING REPRESENTATION OF HEAVY FERMIONIC ATOMS

The quantities of physical interest (density, Green's function etc.) are of the form of a trace with respect to c and f atoms. If $\bar{t}_f = 0$ the Hamiltonian depends only on the integer numbers $\{n_r\}$ and the c operators as

$$H(\{n_r\}) = -\bar{t}_c \sum_{\langle r, r' \rangle} c_r^\dagger c_{r'} + \sum_r \left[n_r (-\mu_f + U c_r^\dagger c_r) - \mu_c c_r^\dagger c_r \right] \equiv -\mu_f \sum_r n_r + H_c(\{n_r\}), \quad (2)$$

where $\bar{t}_c \equiv \bar{t}$ has been used. This means that the f density fluctuations n_r have been replaced by classical variables: $f_r^\dagger f_r \longrightarrow n_r$ which is $n_r = 0, 1$ in the case of fermions. Thus the Green's function can be written as sum over all realizations of n_r as

$$\sum_{\{n_r\}} e^{\beta \mu_f \sum_r n_r} \text{Tr}_c \left(e^{-\beta H_c(\{n_r\})} c_r e^{itH_c(\{n_r\})} c_{r'}^\dagger e^{-itH_c(\{n_r\})} \right).$$

$H_c(\{n_r\})$ is a quadratic form of the c operators. Therefore, it describes independent spinless fermions which are scattered by heavy atoms, represented by n_r . The trace Tr_c in the partition function can be evaluated as a fermion determinant [11]:

$$Z = \sum_{\{n_r\}} e^{\beta \mu_f \sum_r n_r} \text{Tr}_c \left(e^{-\beta H_c(\{n_r\})} \right) = \sum_{\{n_r\}} e^{\beta \mu_f \sum_r n_r} \det[\mathbf{1} + e^{-\beta h_c}]. \quad (3)$$

h_c is an $N \times N$ matrix for N lattice sites with matrix elements $(h_c)_{rr'}$ and there is a distribution $P(\{n_r\})$:

$$(h_c)_{rr'} = -\hat{t}_{rr'} + (U n_r - \mu_c) \delta_{rr'}, \quad P(\{n_r\}) = \frac{1}{Z} e^{\beta \mu_f \sum_r n_r} \det[\mathbf{1} + e^{-\beta h_c}]. \quad (4)$$

The non-negative function $P(\{n_r\})$ gives $\sum_{\{n_r\}} P(\{n_r\}) = 1$ because of Eq. (3). Thus $P(\{n_r\})$ is a probability distribution and the atomic densities are quenched averages with respect to this distribution:

$$n_f = \langle n_r \rangle_f = \sum_{\{n_r\}} n_r P(\{n_r\}), \quad n_{c,r} = \langle [e^{-\beta h_c} (\mathbf{1} + e^{-\beta h_c})^{-1}]_{rr} \rangle_f. \quad (5)$$

3.1. STRONG-COUPLING APPROXIMATIONS FOR THE DISTRIBUTION OF HEAVY FERMIONIC ATOMS

The variables n_r can be expressed by Ising spins $S_r = \pm 1$ as $S_r = 2n_r - 1$. It is possible to discuss the corresponding distribution in terms of magnetic Ising states. This is an extension of the strong-coupling expansion for a fermionic mixture in the symmetric case $\mu_c = \mu_f$ [12].

The strong-coupling expansion of the distribution function $P(\{S_r\})$ in powers of \bar{t}/U gives an expansion in terms of the Ising spins [12,13] with three different regimes:

$$P(\{S_r\}) \propto \begin{cases} \exp \left[\beta \frac{\mu_f}{2} \sum_r S_r \right] & \mu_c < 0 \\ \exp \left[\beta \left(\frac{\mu_f - \mu_c}{2} \sum_r S_r - \frac{\bar{t}^2}{4U} \sum_{\langle r, r' \rangle} S_r S_{r'} \right) \right] & 0 < \mu_c < U \\ \exp \left[\beta \frac{(\mu_f - U)}{2} \sum_r S_r \right] & U < \mu_c \end{cases}. \quad (6)$$

This distribution is a classical Ising model with a magnetic field term $h \sum_r S_r$ and an antiferromagnetic spin-spin interaction $-J \sum_{\langle r, r' \rangle} S_r S_{r'}$ with $J > 0$. The latter is absent in the regimes with $\mu_c < 0$ and $\mu_c > U$. These regimes are only controlled by an effective magnetic field $\mu_f/2$ and $(\mu_f - U)/2$, respectively: A positive field yields a positive Ising spin, implying that the optical lattice is fully occupied by heavy atoms. A negative field yields a negative spin, implying the absence of heavy atoms in the optical lattice. However, there is no real competition between the two atomic species. In the intermediate regime $0 < \mu_c < U$, on the other hand, there is competition due to the appearance of the linear and the bilinear spin terms. The linear term favors a homogeneous distribution of heavy atoms whereas the antiferromagnetic bilinear term favors a staggered distribution of heavy atoms (i.e. a site that is occupied by a heavy atom has nearest neighbor sites without heavy atoms). The latter is caused by the tunneling of the light atoms, since it is proportional to the square of tunneling rate of the light atoms \bar{t} . A simple mean-field calculation reveals that there is a first-order phase transition between the homogeneous phase and the staggered phase. Thermal fluctuations lead to the competition of homogeneous and staggered clusters [12,13]. A typical realization of the distribution of heavy atoms, created by a Monte-Carlo simulation, is shown in Fig. 1. At $\mu_f = \mu_c = U/2$ the distribution in Eq. (4) has a global Ising-spin flip symmetry and is related to a half-filled system. This means that half of the sites of the optical lattice are occupied by heavy atoms. In this case there is a continuous phase transition from antiferro- to paramagnetic order if the temperature is increased.

The complex interplay between light and heavy fermionic atoms in mixtures results in a correlated distribution of the heavy atoms, given by the distribution density of Eq. (4). The correlations are a consequence of the tunneling processes of the light atoms, i.e. they are due to quantum effects.

The symmetric situation $\mu_f = \mu_c$, where the optical lattice does not distinguish between the heavy and the light atoms energetically, there is an additional type of competition

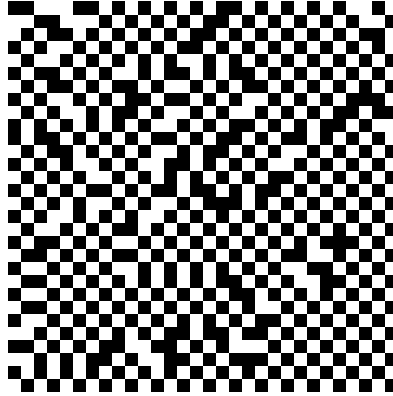


Figure 1. Competition of homogeneous and staggered clusters of heavy fermionic atoms (indicated as dark squares): a typical realization from the distribution in Eq. (4) at $\mu_f = \mu_c = U/2$.

between heavy and light atoms even in the absence of quantum tunneling: although there is no order in the distribution of heavy atoms, the sites of the optical lattice can be randomly occupied either by light or by heavy atoms, provided the repulsion is strong enough (i.e. for $0 < \mu_c = \mu_f < U$). Consequently, the average density is $n_c = n_f = 0.5$. The total symmetric case $\mu_f = \mu_c$ and $\bar{t}_f = \bar{t}_c$ is the Hubbard model. At half-filling the strong-coupling expansion leads to an antiferromagnetic spin-1/2 Heisenberg model [14]. The ground state of this model is a staggered (Neél) state. If the spin is associated with two atomic species, the ground state of the atomic system is an alternating arrangement of the two type of atoms in the optical lattice.

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