

Ground-State Energy and Low-Temperature Behavior of the One-Dimensional Falicov-Kimball Model.

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Abstract. – We consider the Falicov-Kimball model in the case of an equal number of classical «nuclei» and quantum «electrons» with Fermi statistics. In one dimension we find an exact formula for the leading behavior of the ground-state energy as a function of the attractive potential U between electrons and nuclei. For $U > U_c$ the system forms «atoms» which have an effective repulsion between them. Similar results hold for a continuum model provided there is a sufficiently large hard core between the nuclei. Some low-temperature properties are also discussed.

We consider the Falicov-Kimball model as a very primitive model of matter which retains two basic features of electrons and nuclei: the two types of constituents attract each other and the «electrons» are subject to the Pauli principle. The «nuclei» are considered as classical particles with a «hard core», occupying the sites of a lattice \mathbf{Z}^d . The electrons and nuclei interact by an attractive on-site potential. The kinetic energy of an electron is given by the lattice Laplacian $K_{ij} = -\delta_{|i-j|,1} + 2d\delta_{ij}$. For a given configuration of M nuclei the single-electron Hamiltonian has the matrix elements $h_{ij} = K_{ij} - Un_i\delta_{ij}$, $U > 0$, $n_i = 1, 0$ depending on whether the site $i \in \mathbf{Z}^d$ is occupied or not and $\sum n_i = M$. The Hamiltonian of N electrons in such a configuration is the sum $\sum_{\alpha=1}^N h_{ij}^{(\alpha)}$ with Fermi statistics.

Models of this type were discussed in [1, 2] as simplifications of the Hubbard model, in [3] to describe semiconductor-metal transitions and in [4] to study ordering in mixed valence systems. Our interpretation follows Kennedy and Lieb [5, 6] who pointed out that the model can be used to study crystallisation. They and Brandt and Schmidt [7] showed that on cubic (more generally bipartite) lattices, in the *half-filled* state, the nuclei have checkerboard configurations in any dimension for zero temperature and in dimension greater than one for low temperatures. This long-range order is destroyed at high temperatures and the correlations fall off exponentially. Details of this Ising-like transition have been worked out in the limit of high dimension [8, 9] and an exact solution found for infinite dimension [10].

Here we consider the one-dimensional case. We shall be mainly concerned here with the nature of the ground state for the case of an equal number of nuclei and electrons. For a given configuration of M nuclei the ground-state energy of N electrons will be denoted by $E((l)_M, N)$, where $(l)_M$ denotes the set of successive distances, number of empty sites, (l_1, \dots, l_{M-1}) between the nuclei. If $M = 1$ there is a unique one-electron bound state, «the atom», with energy $E_{\text{at}} = 2 - (U^2 + 4)^{1/2} \equiv 2 - \varepsilon - \varepsilon^{-1}$, $\varepsilon \in [0, 1]$, and wave function $\psi_{\text{at}}(i) \sim \varepsilon^{|i|}$.

We prove, for the neutral case $N = M$, that there exists a U_c such that for $U > U_c$ (or $\varepsilon < \varepsilon_c < 1$)

$$E((l)_N, N) = NE_{\text{at}} + \left[\sum_{i=1}^{N-1} 2(l_i + 1) \varepsilon^{2l_i + 1} \right] (1 + \sqrt{\varepsilon} R(\varepsilon, (l)_N)) \quad (1)$$

with the remainder term $R(\varepsilon, (l)_N)$ bounded by a constant C which, like U_c , is independent of N, l_1, \dots, l_{N-1} . This implies that we can take the thermodynamic limit of (1)

$$\lim_{N \rightarrow \infty} \frac{1}{N} E((l)_N, N) = E_{\text{at}} + \text{Av}[\phi(l)(1 + O(\sqrt{\varepsilon}))], \quad (2)$$

where $\phi(l) = 2(l + 1) \varepsilon^{2l + 1}$ and Av denotes the average with respect to the distribution of distances between the nuclei.

Equation (1) implies that for $U > U_c$ an equal number of electrons and nuclei will form atoms (rather than molecules) with an energy equal to $\min_{(l)_N} E((l)_N, N) = NE_{\text{at}}$. There will be an effective repulsion between adjacent atoms and on an infinite lattice they will spread out to infinity. The minimum of the potential energy function $\sum_i \phi(l_i)$ under the constraint $\sum_i l_i = (N - 1)l$ is attained for uniform spacing, $l_i = l$. The configuration of nuclei, constrained

to be in a fixed region, will thus likely tend to be periodic for $U > U_c$. For an infinite system of density n we expect the atoms to have a uniform spacing $l = n^{-1} - 1$ between them, which then leads to an energy per atom equal to $E_{\text{at}} + (2/n\varepsilon) \varepsilon^{2/n} (1 + O(\sqrt{\varepsilon}))$. This uniform-spacing property was conjectured in [11] and a result of this type has in fact been established [12] for $U > U_{\text{min}}$. However this U_{min} (unlike our U_c) depends on the density of nuclei and tends to infinity as the density vanishes.

Both the Fermi statistics and the neutrality condition play a crucial role in the structure of the ground state. Indeed if the electrons were bosons the nuclei would clump together [5]; moreover, even for fermions Freericks and Falicov [11] argued that when the density of electrons is appreciably lower than that of nuclei (depending on U) these could clump together. This is the so-called segregation principle which has been proved for some range of parameters [12] (see also [13]).

We note that the dominant part of the second term in (1) is a sum of potentials $\phi(l_j)$ between nearest-neighbor nuclei separated by l_j empty sites on the lattice. Using $\phi(l)$ as an approximate potential between adjacent atoms at low temperature, we can compute the thermodynamics of this system. For a fixed density, this is a legitimate procedure if the temperature is sufficiently low. Indeed it is known that for $U > 4$ there is a gap greater than or equal to $U - 4$, between the ground state of N electrons in any given configuration of N nuclei and the excited states. Using the pressure ensemble, the equation of state is easily found to be $\beta n^{-1} = -(\partial/\partial p) \ln Z(p)$ with

$$Z(p) = \sum_{l=0}^{\infty} \exp[-\beta[p(l + 1) + \phi(l)]], \quad (3)$$

where n is the density of atoms and p the pressure. For small ε and fixed density we have $n^{-1} \approx (1 - \exp[-\beta p])^{-1} + 2\varepsilon\beta \exp[-\beta p]$ which is the equation of state of a free lattice gas of atoms with repulsive interaction $\phi(l)$.

We remark that the results of [5, 14] are consistent with the assumption that there is a similar nearest-neighbor repulsion between the atoms in dimensions greater than one. In fact a formal large U expansion [14] shows that the model behaves to leading order like an Ising antiferromagnet with exchange constant $1/2U$ and magnetic field $(\mu_e - \mu_n)/2 - d$, (μ_e, μ_n) being the chemical potentials of the electrons and nuclei. This is consistent with (1). By accepting this, then for values of the chemical potentials such that the corresponding magnetic field is sufficiently small compared to its critical value, the phase diagram of the Falicov-Kimball model ought to look similar to that of an Ising antiferromagnet with the critical exponents of the half-filled state being of the standard Ising type. So far the investigation of the phase diagram at nonzero temperature has received a rigorous treatment only when $\mu_e = 2d - U/2$, $\mu_n = -U/2$ corresponding to half-filling [5]. For zero temperature the domain of chemical potentials corresponding to the checkerboard state has been identified as a strip (of width $1/U$ for large U) around the segment $\mu_e + \mu_n = 2d - U$, $4d - U < \mu_e < 0$ [14].

For fixed positive temperature and $n \rightarrow 0$ it is not legitimate to use the effective interatomic potential $\phi(l)$ directly because the entropy contribution of the positive-energy states of the electrons, which correspond in fact to «ionised» electrons, becomes important. Instead one has to start with the full partition function of the Falicov-Kimball model which yields in this limit $\beta p \approx 2n$. (Note that the direct use of (3) would give a wrong answer, namely $\beta p \approx n$.) We therefore see that in this limit the electrons and nuclei do not bind to form atoms but are «ionised». This is also the case for real Coulombic matter [15].

We now consider the behavior of the system at low temperature for values of μ_e, μ_n where the density goes to zero as $\beta \rightarrow \infty$ (for $U > 4$, this is the case in the domain $\mu_e + \mu_n < -U$, $\mu_n < -4$, see [14, 16]). The simplest way to identify the phases of the system in this domain is by looking at the asymptotic behavior of the equation of state. Using the grand canonical ensemble, we see that the system will form an atomic gas as $\beta \rightarrow \infty$ for those values of μ_e, μ_n for which

$$E((l)_M, N) - \mu_e N - \mu_n M > E_{\text{at}} - \mu_e - \mu_n > 0 \quad (4)$$

is satisfied for all $(N, M) \neq (0, 0)$ and $(1, 1)$. Such values of μ_e, μ_n will exist if the system satisfies a stability condition with a «good constant»: there exists a constant K , $0 < K < |E_{\text{at}}|$ such that $\min_{(l)_M} E((l)_M, N) > -K(N + M - 1)$, for $N + M > 2$. When this is the case the system forms an ideal gas of atoms for $\beta \rightarrow \infty$ and μ_e, μ_n fixed in the square $E_{\text{at}} < \mu_e, \mu_n < -K$. On the other hand for $\mu_e < \mu_n < -K, \mu_e < E_{\text{at}}$ the system consists of free nuclei and for $\mu_n < \mu_e < -K, \mu_n < E_{\text{at}}$ it consists of free electrons. At the common boundaries of these domains there exists a whole continuum of partially ionised phases with degrees of ionisation given by Saha-type formulae.

The above analysis is adapted from investigations of the low-temperature-low-density behavior of real matter [17-19]. We note that, while it is not yet proven that there exist $K < |E_{\text{at}}|$ for the true Coulombic case, it is easy to do so for this model. Indeed if $N \leq M$, because of the Fermi statistics $E((l)_M, N) \geq NE((l)_M, 1)$ for any configuration $(l)_M$. Since the spectrum of the single-electron Hamiltonian is bounded below by $-U$ we have $\min_{(l)_M} E((l)_M, N) \geq -NU$. Moreover, for $N \leq M$ and $N + M > 2$ we have $N < 3(N + M - 1)/4$, which gives $K = 3U/4$ for this case. If $N > M$, $E((l)_M, N) > E((l)_M, M)$ and the problem is reduced to the previous case. The last inequality follows from the Fermi statistics together with the fact that for any configuration $(l)_M$ the number of negative eigenvalues of the

single-electron Hamiltonian is M . With the choice $K = 3U/4$ the inequality $K < |E_{\text{at}}|$ is satisfied for $U > 8$. Thus for $U > 8$ we get an atomic gas for a range of chemical potentials indicated above. This of course is not an optimal result. In fact our theorem implies that we can choose the better value $K = 3|E_{\text{at}}|/4$ for $N \geq M$. For $N = M$ we obtain the optimal value $K = 2|E_{\text{at}}|/3$. Unfortunately, we do not have good information for $N < M$. Finally let us note that from (1) it is clear that the system cannot possibly form a gas of «neutral» entities other than atoms (for example molecules with two nuclei and two electrons) but because of the segregation phenomenon one can expect that gases of «non-neutral» entities can form in this model for other values of the chemical potentials.

In the rest of this note we sketch the proof of (1). The first step is to derive a polynomial equation for the eigenvalues of the one-electron Schrödinger equation $\sum_j h_{ij} \Psi(j) = E\Psi(i)$. The bound states are of the form

$$\Psi(i) = A_i(\varepsilon y)^i + B_i(\varepsilon y)^{-i},$$

where y is related to their energy by $E = 2 - \varepsilon y - 1/\varepsilon y$, $0 < \varepsilon y < 1$. Here $A_i = 0$, $B_i = B$ for all $i < i_l$, the position of the left-most nucleus, and $B_i = 0$, $A_i = A$ for all $i > i_r$, the position of the right-most nucleus. Note that if the site i is empty $A_{i-1} = A_i$, $B_{i-1} = B_i$. By introducing the transfer matrix T_i , the condition for Ψ to be a bound state reduces to $(0, B) = T_{i_l} \dots T_{i_r+1}(A, 0)$. This means that the matrix element $[T_{i_l} \dots T_{i_r+1}]_{11}$ must vanish and leads to the equation

$$0 = P_N(y, (l_N)) \equiv \left[\prod_{i=1}^N Q(l_i) \right]_{11} \quad (5)$$

with the matrix $Q(l)$ given by

$$\begin{pmatrix} (1-y)(1+\varepsilon^2 y) & -\varepsilon^{-2}(1-\varepsilon^2)^2(\varepsilon y)^{2l+4} \\ 1 & (1+y)(1-\varepsilon^2 y)(\varepsilon y)^{2l+2} \end{pmatrix}.$$

In (5) P_N is a polynomial in the variable y and has the degree $\sum_{i=1}^{N-1} (2l_i + 4) > N$ for $N > 1$ (note that the result is independent of L_N which is arbitrary). The ground-state energy is given by $\sum(2 - \varepsilon y_k - 1/\varepsilon y_k)$, where the sum is over the N physical roots of the polynomial (*i.e.* y real and $0 < \varepsilon y < 1$).

We are now faced with the problem of determining the location of the physical roots of P_N in the complex plane. For $U > 4$ ($\varepsilon < 0.236$) and N nuclei the one-electron Hamiltonian has N eigenvalues contained in the interval $E \in [-U, 4 - U]$. The relation between E and y then shows that P_N must have N physical roots contained in the interval $y \in [0.8, 1.5]$ as long as $\varepsilon < 0.14$ ($U > 7$). For one nucleus $N = 1$, (5) reduces to $P_1(y) = (1-y)(1+\varepsilon^2 y) = 0$. The physical solution $y = 1$ yields $E_{\text{at}} = 2 - (\varepsilon + \varepsilon^{-1})$. The polynomial has a general factorisation property: if $l_k \rightarrow \infty$ then P_N tends to

$$P_k(y, l_1 \dots l_{k-1}) P_{N-k}(y, l_{k+1} \dots l_{N-1}),$$

and thus P_N tends to $(P_1(y))^N$ when all $l_i \rightarrow \infty$. This is also the case when $\varepsilon \rightarrow 0$ and indicates that the N physical roots should concentrate around 1 as $\varepsilon \rightarrow 0$ or all $l_i \rightarrow \infty$. We explain later how to prove that for $\varepsilon < \varepsilon_c$ there exist *exactly* N roots in the interval $|y - 1| < \varepsilon^{(l_m + 1/2)/2}$, where l_m is the smallest distance between nuclei. Moreover all other (nonphysical) roots of P_N are located in the complex plane outside a disc of center 1 and radius $1/2$.

Our result is based on Cauchy's formula

$$E((l)_N, N) = \int_C \frac{dz}{2\pi i} \left[2 - \varepsilon z - \frac{1}{\varepsilon z} \right] \frac{P'_N(z, (l)_N)}{P_N(z, (l)_N)}$$

with the contour C a circle included in the annulus $\varepsilon^{(l_m + 1/2)/2} < |1 - z| < 1/2$, so that it encloses all the physical roots and only these ones. The relation $P'_N/P_N = (\ln P_N)'$ suggests that we view P_N as a kind of partition function of some classical system. Defining two functions $\zeta(y, l)$ and $w(y)$ by $\zeta(y, l) = Q_{12}(l)/(P_1(y))^2$ and $\zeta(y, l)w(y) = Q_{22}(l)/P_1(y)$, we can write the polynomial as

$$P_N = (P_1(y))^N \left[\prod_{i=1}^{N-1} (1 + \zeta(y, l_i)) \right] Z_N(y, (l)_N)$$

with $Z_N(y, (l)_N)$ equal to

$$\sum_{\{n_i=0, 1\}} \prod_{i=1}^{N-1} \frac{(\zeta(y, l_i))^{n_i}}{1 + \zeta(y, l_i)} \prod_{i=1}^{N-2} w(y)^{n_i n_{i+1}},$$

the partition function of a lattice gas on $N - 1$ sites which are occupied with probability $\zeta(y, l_i)/(1 + \zeta(y, l_i))$ and have nearest-neighbor interaction determined by the function $w(y)$.

The ground-state energy of the one-dimensional quantum model can then be related to the «free energy» $F(y, (l)_N) = \ln Z_N(y, (l)_N)$ associated with this one-dimensional classical model by

$$E((l)_N, N) = NE_{\text{at}} + \sum_{i=1}^{N-1} \int_C \frac{dz}{2\pi i} \left[2 - \varepsilon z - \frac{1}{\varepsilon z} \right] \frac{\zeta'(z, l_i)}{1 + \zeta(z, l_i)} + \int_C \frac{dz}{2\pi i} \left(2 - \varepsilon z - \frac{1}{\varepsilon z} \right) \frac{d}{dz} F(z, (l)_N). \quad (6)$$

We observe that $\zeta'/(1 + \zeta) = P'_2/P_2 - 2P'_1/P_1$, which means that the terms of the sum in (6) are equal to $E(l_i, 2) - 2E_{\text{at}}$. This is the effective two-body repulsive potential between a pair of nuclei separated by a distance l_i . An explicit computation shows that it is equal to $\phi(l_i) \cdot (1 + O(\varepsilon^2))$, where $O(\varepsilon^2)$ is a term bounded by $C\varepsilon^2$ for a constant C independent of N and $(l)_N$. The third term on the right-hand side of (6) involves the corrections given by the n -body effective potentials between n nuclei. A systematic perturbation series for this term, with known bounds (three graph bounds) for all orders, is provided by the polymer expansion developed for spin systems [20, 21]. This enables us to show that it is bounded by $C\varepsilon^{1/2} \sum_i \phi(l_i)$ for $\varepsilon < \varepsilon_c$, where C is a constant independent of $N, (l)_N$.

To control the location of the roots of P_N , we first use the polymer expansion to prove the analyticity of $F(z, (l)_N)$ in the annulus $\varepsilon^{(l_m + 1/2)/2} < |1 - z| < 1/2$ for $\varepsilon < \varepsilon_c$. Then as a consequence of Cauchy's formula for the number of roots of a polynomial inside a contour C of the complex plane we deduce that any C contained in this annulus encloses exactly N roots of P_N . Moreover, we already know that N physical roots are contained in an interval around one for small ε . Thus C encloses only these ones.

The same technique can be used to prove a result similar to (1) for a continuous analog of the Falicov-Kimball model. The electrons and nuclei now move on the real line and the nuclei have a mutual repulsion corresponding to hard rods of length h . The nuclei and electrons

attract each other with the local potential $-\gamma\delta(r)$, $\gamma > 0$. The only dimensionless parameter now is $\gamma h \equiv a$. Our results then show that there exists an a_c independent of the nuclei's configuration such that for $a > a_c$ a formula similar to (1) with E_{at} replaced by $-\gamma^2/4$ and $\phi(l)$ replaced by $\exp[-\gamma l](\gamma l - 1)\gamma^2/2$, $l > h$. Thus as for the lattice model the ground state consists of atoms with an effective repulsion between them. For a sufficiently small value of a the structure of the ground state can be very different. Indeed in the case of two electrons and two nuclei one can show that for small a the system prefers to form a bound state with two nuclei and one electron, the other one being itinerant. For intermediate values of a the ground state corresponds to both electrons being bound to a pair of nuclei with minimal distance between them.

Finally let us note that although our analysis is limited to one dimension we expect that the nature of the ground state is similar in the case of higher-dimensional lattices. Indeed perturbation series in $1/U$ [16] suggest that in the *neutral* case the effective interaction (induced by the Fermi statistics) is repulsive.

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