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# Spinless Fermi Gas on One-Dimensional Lattice : Rigorous Results

Ch. Gruber
Institut de Physique Théorique
Ecole Polytechnique Fédérale de Lausanne
PHB-Ecublens - CH-1015 Lausanne, Switzerland

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Abstract

The ground state configurations of the one-dimensional Fermi gas (Falicov-Kimball model) are investigated using expansion in powers of $U^{-1}$, where U is the interaction strength. For a given ion density $\rho_i = \frac{p}{q}$ we consider only those periodic configurations defined by $\nu p$ ions followed by $\nu(q-p)$ holes. We then show that there exists critical values $\rho_e'$ and $\rho_e''$ such that for electron densities $\rho_e < \rho_e'$ the segregated configuration ($\nu = \infty$) has lowest energy (in the family of configurations under consideration), while for $\rho_e'' < \rho_e \leq 1 - \rho_i$ (or $\rho_e'' \leq \rho_e \leq \rho_i$ if $U < 0$) it is the configuration with period q ($\nu = 1$). In particular the segregated configuration cannot be a ground state for $\rho_e > \rho_e''$.

## 1. Introduction

The Falicov-Kimball model can be viewed as a lattice model of spinless quantum electrons interacting with classical ions. The electrons do not interact with each other, and the only interaction between ions is a point hard-core (i.e. the sites of the lattice are either empty or occupied by a single ion). The energy of the system is simply the sum of the kinetic energy of the electrons and the interaction energy between ions and electrons.

The Hamiltonian is

$$H = -\sum_x \left(a_x^+ a_{x+1} + a_{x+1}^+ a_x\right) + U \sum_x a_x^+ a_x W(x)$$

where $a_x^+$, $a_x$ are the creation and annihilation operators for a spinless electron at site x, W (x) is 1 or zero according to whether the site x is occupied by an ion or empty.

This model was originally introduced to study metal-insulator transitions in transition-metal oxides [1]. Later it was realized that the same model is also of interest to study crystallization and mixed-valence phenomena [2, 3]. It is also a simplified version of the Hubbard model [2].

The problem one would like to consider is the following : given the ion and electron densities $\rho_i$, $\rho_e$, what is the configuration of ions for which the energy of the system is minimum (= ground state configuration) ?

In a recent work, Freericks and Falicov [4] arrived at a conjecture which is very interesting, but also very surprising : if the interaction is attractive ($U < 0$), then for $\rho_e = \rho_i$ the ground state configuration is periodic with maximum possible spacing between ions (which corresponds to a repulsive effective interaction between ions), on the other hand for $\rho_e < \rho_e^c < \rho_i$, (where the critical value $\rho_e^c$ depends on the interaction U, and the ion density $\rho_i$) the ground state configurations is the "segregated configuration" where all ions clump together. For densities between $\rho_e^c$ and $\rho_i$, the situation is highly complex : it is expected that an infinite number of transitions, with a devil's staircase structure, will appear, with ground state configurations which are periodic or mixtures. Finally it is conjectured that $\rho_e^c$ tends to $\rho_i$ as $U \to \infty$. If the interaction is repulsive ($U > 0$) the

conjecture is similar replacing "ions" by "holes", i.e. for $\rho_e = 1 - \rho_i$ the ground state configuration is periodic, while for $\rho_e < \rho_e^c < 1 - \rho_i$ the segregated configuration gives the minimum energy.

In this article, we establish results which tend to support the above conjecture. Given the ion and electron densities $\rho_i, \rho_e$, we consider only crenel configurations defined by clusters of m ions separated by the distance a (fig. 4), and we look for the size of the clusters for which the energy is minimal. We then show that for attractive interaction ($U < 0$) the size of the cluster is minimal if $\rho_e = \rho_i$; furthermore there exist $\rho_e^c$ such that if $\rho_e < \rho_e^c$ then the segregated configuration has minimal energy (among crenel configurations); finally for $\rho_e^c < \rho_e < \rho_i$ the configuration defined by the mixture of the periodic configuration (corresponding to $\rho_e = \rho_i$) and the segregated configuration has energy which is smaller than both the segregated and the periodic. For the repulsive case ($U > 0$), if $\rho_e = 1 - \rho_i$ the size of the cluster is minimal; furthermore there exists $\rho_e^c$ such that for $\rho_e < \rho_e^c$ the segregated configuration has minimal energy; for $\rho_e^c < \rho_e < 1 - \rho_i$, the mixture of segregated and periodic configuration has energy smaller than both.

In Section 2, we define the model and present a qualitative discussion of the transition between the segregated and the periodic configurations. Then, in the subsections of Section 3, we are concerned with crenel or segregated configurations. These configurations are defined in sect. 3.1; the method we have used is based upon the expansions in power of $U^{-1}$ for the eigenvalues (sect. 3.2) and for the ground state energy (sect. 3.3). To establish our main results (sect. 3.5), we need bounds to estimate the rest of the expansions and this is done in sec. 3.4. In the last Section, we conclude with some remarks which are valid for arbitrary configurations. In particular, for the ion density $\rho_i = \frac{1}{q}$ (q = integer), it is shown that the periodic configuration with period q can be a true ground state configuration only if the electron density $\rho_e$ is equal to $\rho_i$ (if the interaction is attractive); for repulsive interaction and $\rho_i = 1 - \frac{1}{q}$ the periodic configuration with period q can be a true ground state only if $\rho_e = \frac{1}{q}$.

## 2. Qualitative discussion

The general picture recently discovered by Freericks and Falicov [1] can be qualitatively understood using simple properties of the Fermi energy, at least if the coupling constant U satisfies the condition $|U| > 4$, which is the case we want to study in this paper.

We consider a system consisting of $N_i$ ions and $N_e$ electrons on a one-dimensional regular lattice $\Lambda$ with N sites and periodic boundary conditions. We denote the ion configurations by $s = \{s_x \mid x \in \Lambda\}$, where the variable $s_x$ is + 1 if the site is occupied by an ion and - 1 if it is empty. Since the electrons do not interact with each other the Fermi energy is obtained by filling the lowest $N_e$ levels of the one-electron Schrödinger equation on the lattice,

$$-[\psi_n(x+1) + \psi_n(x-1)] + U(x)\,\psi_n(x) = E_n\,\psi_n(x) \tag{1}$$

where :

$$U(x) = U\,\frac{s_x + 1}{2} = \begin{cases} U & \text{if } x \text{ is occupied} \\ 0 & \text{if } x \text{ is empty} \end{cases}$$

and $$E_n \in [-2, +2] \cup [U-2, U+2]$$

Let $$E_N(U, \rho_e; s) = \frac{1}{N} \sum_{n=1}^{N_e} E_n \tag{2}$$

denote the <u>ground state energy</u> (per lattice site) for the configuration s, with

$$\rho_e \equiv \frac{N_e}{N} \quad , \quad \rho_i \equiv \frac{N_i(s)}{N} \tag{3}$$

the electron and ion densities.

Given $(U, \rho_e; \rho_i)$, the problem is then to find the ion configuration s, with $\rho_i(s) = \rho_i$, which minimize (2), i.e.

$$E_N(U, \rho_e; \rho_i) \equiv E_N(\rho_e) \equiv \min\{E_N(U, \rho_e; s) \mid \rho_i(s) = \rho_i\} \tag{4}$$

We call <u>ground state configuration</u> (gsc) for the densities $(\rho_e, \rho_i)$, those ions configurations for which the minimum in (4) is obtained, and denote by $G(\rho_e, \rho_i)$ the family of all gsc for $(\rho_e, \rho_i)$.

Let us recall that the function $E_N(\rho_e)$ is continuous, convex, differentiable almost everywhere with slope given by the Fermi level. Furthermore, using the particle-hole symmetry, one has the following identities [1] :

$$E_N(U, \rho_e; s) = E_N(-U, \rho_e; -s) + U\rho_e \tag{5}$$

$$E_N(U, \rho_e; s) = E_N(U, 1-\rho_e; -s) + U(\rho_e + \rho_i - 1) \tag{6}$$

We shall thus restrict ourselves to the repulsive case $U > 0$. (The attractive case $U < 0$ is identical if we interpret $s_x = +1$ as an empty site and $s_x = -1$ as occupied). On the other hand Eq. 6 implies

$$E_N(U, \rho_e; \rho_i) = E_N(U, 1-\rho_e; 1-\rho_i) + U(\rho_e + \rho_i - 1) \tag{7}$$

and we can restrict the discussion to the case $\rho_e \leq 1 - \rho_i$ (which is $\rho_e \leq \rho_i$ for $U < 0$). To simplify the qualitative discussion, we shall consider the thermodynamic limit $N \to \infty$, with fixed $(\rho_e, \rho_i)$, and periodic ion configurations s such that $\rho_i(s) = \rho_i$. The energy levels $E_n = E_n(U; s)$ are non decreasing as U increases. Therefore, for a given s and $\rho_e$, the ground state energy Eq. 2 is an increasing function of U; moreover for any $\tilde{\rho}_e > \rho_e$ we have

$$E_N(\infty, \tilde{\rho}_e; s) - E_N(U, \tilde{\rho}_e; s) \geq E_N(\infty, \rho_e; s) - E_N(U, \rho_e; s) \geq 0$$

Furthermore

$$\begin{aligned} \frac{\partial E_N}{\partial \rho_e}(U, \rho_e = 0; s) &= E_1(U; s) \geq -2 \\ \frac{\partial E_N}{\partial \rho_e}(U, \rho_e = 1-\rho_i; s) &= E_{n=N-N_i}(U; s) \leq 2 \end{aligned} \tag{8}$$

and both derivatives are non decreasing as U increases.

Finally, let us remark that given N, $\rho_i$, $\rho_e$ and $U = \infty$, then the ion configuration which minimizes Eq. 4 is the segregated configuration (= seg) where all ions clump together ($U(x) = U$ for $1 \le x \le N_i$ and $U(x) = 0$ for $N_i < x \le N$). In the thermodynamic limit the ground state energy for the segregated configuration is given for all $U \ge 4$ by

$$E_{seg}(U,\rho_e;\rho_i) = -\frac{2}{\pi}(1-\rho_i)\sin\left(\pi\frac{\rho_e}{1-\rho_i}\right) \qquad \text{for } \rho_e \le 1-\rho_i$$

$$E_{seg}(U,\rho_e;\rho_i) = -\frac{2}{\pi}\rho_i \sin\left(\pi\frac{1-\rho_e}{\rho_i}\right) + U(\rho_e+\rho_i-1) \qquad \text{for } \rho_e \ge 1-\rho_i \tag{9}$$

(For $U = \infty$, then $\rho_e \le 1 - \rho_i$ and the above result is straightforward; for $U < \infty$ see Sec. 3.4)

The consequences of these general properties are shown in figure 1 for large U (the ion density for the segregated configuration is $\rho_i = \rho_i$ (s)), and yield the following :

1) For $\rho_e < \rho_e'$ (s) the segregated configuration has lower energy then s, while for $\rho_e > \rho_e'$ (s) it cannot be a gsc. Moreover $\rho_e'$ (s) is an increasing function of U which tends to $(1 - \rho_i)$ as $U \to \infty$.

2) Let $s_o$ be a gsc for $\rho_e = 1 - \rho_i$ (fig. 3). Constructing the convex envelope of the functions $E(U, \rho_e; s_o)$ and $E(U, \rho_e; \text{seg})$, we see that for values of $\rho_e$ corresponding to the linear part of this envelope, i.e. $\rho_e > \rho_e^c$, the configuration represented in figure 2 has an energy which is lower than the energies of both the segregated and $s_o$ configurations : it is a mixture of the segregated and $s_o$ configurations.

3) We shall see below (Proposition 5) that for large U, the convex envelope may coincide with $E(U, \rho_e; s_o)$ only at $\rho_e = 1 - \rho_i$. In this case $s_o$ is a gsc only for $\rho_e = 1 - \rho_i$. For $\rho_e^c < \rho_e < (1 - \rho_i)$ the mixture configuration has energy smaller than seg. and $s_o$; for $\rho_e \le \rho_e^c$ the segregated configuration has energy smaller than $s_o$ and mixture. Moreover $\rho_e^c$ is an increasing function of U which tends to $(1-\rho_i)$ as $U \to \infty$.

4) If there exists $\rho_e' > 0$ such that $\rho_e'(s) \geq \rho_e'$ for any periodic configuration s, then for $\rho_e < \rho_e'$ the gsc cannot be periodic. In this case constructing the convex envelope, we conclude that there exists $\rho_e^{(c)}$ such that for $\rho_e < \rho_e^{(c)}$ the segregated configuration has energy smaller than any periodic configuration, while for $\rho_e^{(c)} \leq \rho_e < 1 - \rho_i$, the ground state configurations are either periodic, or mixture of two periodic configurations (or some other configurations which cannot be obtained by means of periodic configurations).

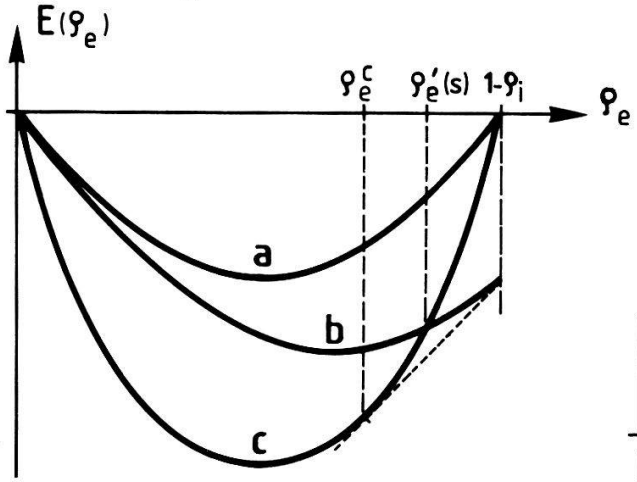


Fig. 1.
a) $E(U = \infty, \rho_e; s)$
b) $E(U, \rho_e; s)$
c) $E(U, \rho_e; seg) = E(\infty, \rho_e; seg)$ for all $U > 4$.

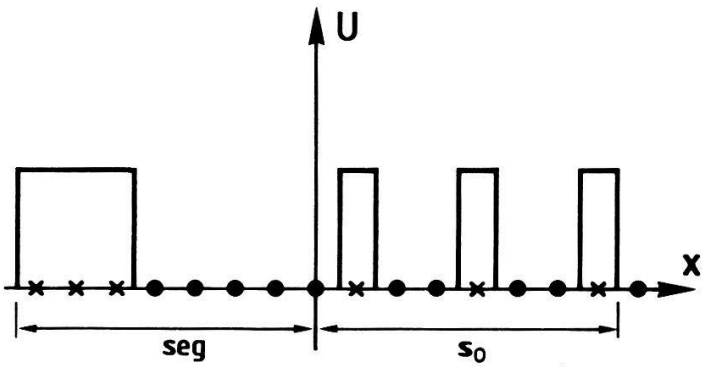


Fig. 2. Mixture of $s_0$ and segregated

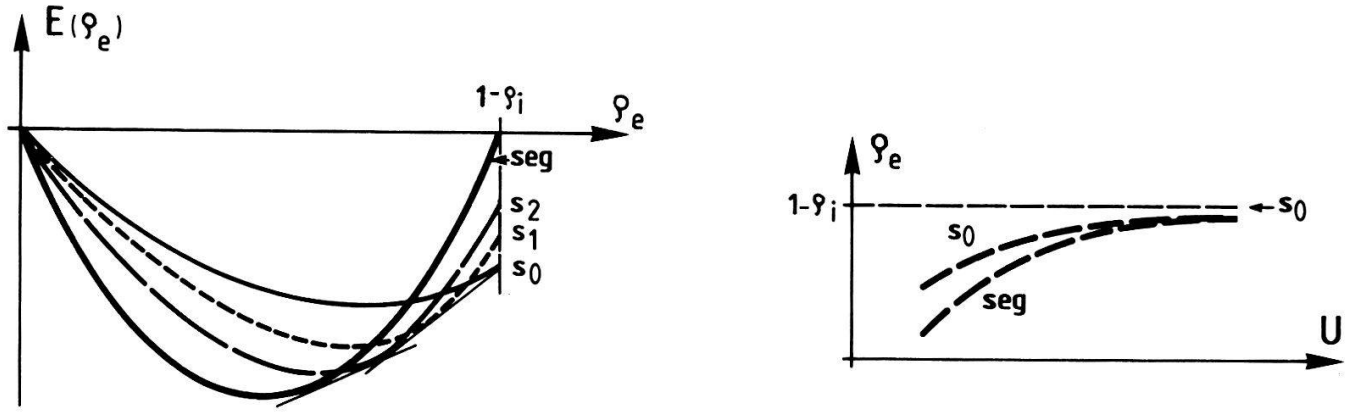


Fig. 3. Ground state configurations for a given ion density $\rho_i$

## 3. Crenel configurations

### 3.1. Definitions

In the following, we consider only crenel configurations, i.e. periodic square barrier potentials U(x) with width m and separation a (fig. 4).

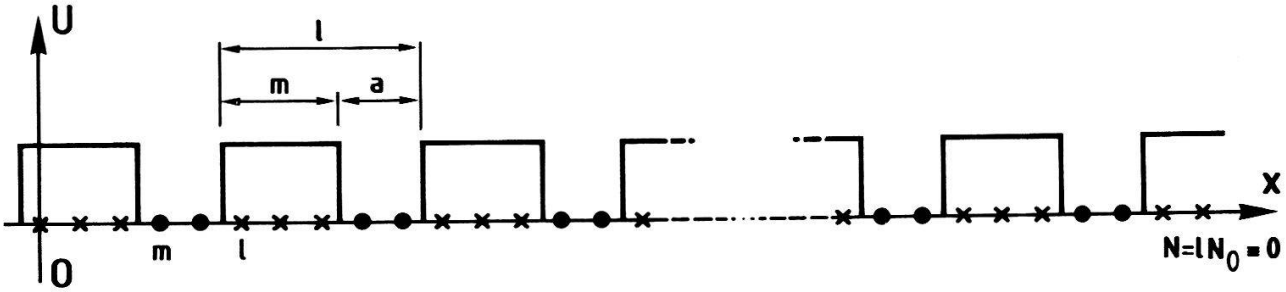


Fig 4. Crenel configuration with ion density $\rho_i = \frac{m}{l}$.

For a given ion density

$$\rho_i = \frac{p}{q} \tag{10}$$

with p relatively prime to q, we shall then consider those crenel configurations with $N = l \cdot N_o$ sites,

$$l = \nu q \quad , \; m = \nu p \quad , \; a = \nu(q-p) = \nu q\,(1 - \rho_i)\,, \tag{11}$$

where $\nu$ is an integer, and $N_o \to \infty$ in the thermodynamic limit. The condition $\rho_e \leq 1 - \rho_i$ is expressed by

$$N_e \leq N - N_i = N_o\ \nu\ \ (q-p) = (1 - \rho_i)\ N_o\, l. \tag{12}$$

The problem we want to study is the following : given $\rho_i$ and $\rho_e$, for what values of $\nu$ is the ground state energy minimal ?

Let us recall that for any configuration of ions, and $U > 4$, there are exactly $N-N_i$ eigenvalues in $[-2, +2]$ (Gerschgorin's theorem, Bull. Acad. Sc. Leningrad 1921, 749-754).We introduce the notation

$$E_n = -2\cos k = U - 2\,\mathrm{ch}\,\kappa \tag{13}$$

For the following discussion, we note that

$$\exp(-\kappa) = \frac{1}{2}\left\{(U-E_n) - \sqrt{(U-E_n)^2 - 4}\right\} = O\left(U^{-1}\right) \tag{14}$$

### 3.2. Asymptotic Expansion for the Eigenvalues

Using standard techniques, we obtain the eigenvalue equation

$$\cos(l\,K)\;[\mathrm{ch}(m\kappa)]^{-1}\sin k = \sin\big((a+1)k\big) - \varepsilon(k)\sin(a\,k)$$

$$l\,K = \frac{2\pi}{N_o}\{1,\ldots,N_o\} \tag{15}$$

where

$$\varepsilon(k) = \frac{\mathrm{th}\,(m\kappa)}{\mathrm{sh}\,(\kappa)}\left[1+\frac{1}{4}E_n(U-E_n)\right] - \frac{1}{2}E_n\,. \tag{16}$$

To discuss the asymptotic expansion with respect to $U^{-1}$ we rewrite $\varepsilon(k)$ in the form :

$$\varepsilon(k) = \left[1+e^{-2m\kappa}\right]^{-1}\left\{B - \frac{e^{-2m\kappa}}{1-e^{-2m\kappa}}\left(2\,e^{-\kappa}+E_n\right)\right\} \tag{17}$$

$$B = \frac{e^{-\kappa}}{1-e^{-2\kappa}}\,(2+E_n\,e^{-\kappa}) = O\,(U^{-1}) \tag{18}$$

or equivalently

$$\varepsilon\,(k) = \frac{1-e^{-2m\kappa}}{1+e^{-2m\kappa}}B - \frac{e^{-2m\kappa}}{1+e^{-2m\kappa}}E_n \tag{19}$$

For $U = \infty$ , Eq. (15) yields

$$\sin\big((a+1)\,k\big) = 0\ ,\ \text{i.e. } k_n^{(\infty)} = \frac{n\,\pi}{a+1}\quad ,\ n = 1,\ldots,a.$$

Since $E_n$ is non-decreasing as U increases, we introduce $\delta_n$ which describes the correction to $k_n$ with respect to $\frac{n\,\pi}{a+1}$ , i. e.

$$E_n = -2\cos\left(\frac{n\,\pi-\delta_n}{a+1}\right) \tag{20}$$

where $\delta_n \geq 0$: $\delta_n$ satisfies the equation

$$\sin \delta_n = \varepsilon(\delta_n) \sin\left(\frac{n\pi + a\delta_n}{a+1}\right) + \\ + \cos(l\,K)\,[\mathrm{ch}(m\kappa)]^{-1} \sin\left(\frac{n\pi - \delta_n}{a+1}\right) \tag{21}$$

$$\varepsilon(\delta_n) = \varepsilon(k) \quad \text{with} \quad k = \frac{n\pi - \delta_n}{a+1}, \quad n = 1, \ldots, a.$$

We should remark that for the single potential well (fig. 5) we have

$$\sin \delta_n = B(\delta_n) \sin\left(\frac{n\pi + a\,\delta_n}{a+1}\right)$$

with B given by Eq. 18. From Eqs, 21, 19, we see that the corrections with respect to the single potential well are of the order $U^{-m}$ as $U \to \infty$.

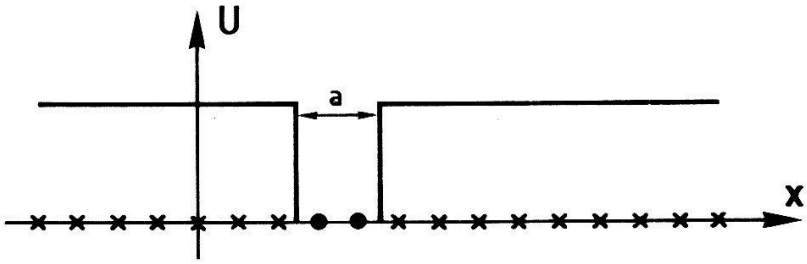


Fig. 5 Potential well

Let us also note that for m = 1, Eq. (21) becomes

$$\sin \delta_n = [\mathrm{ch}\,\kappa]^{-1} \left\{\sin\left(\frac{n\pi + a\delta_n}{a+1}\right) + \cos(l\,K) \sin\left(\frac{n\pi - \delta_n}{a+1}\right)\right\} \tag{22}$$

and thus for cos (l K) = - 1 we have $\delta_n = 0$. For any other value of cos (l K)

$$\delta_n < \pi/2 \quad , \text{ if } U \geq 6.$$

For m > 1, Eqs. 19 and 18 imply

$$|\varepsilon(k)| \leq |B| + e^{-m\kappa}[\mathrm{ch}\,m\kappa]^{-1} \leq 2\,\frac{e^{-\kappa}}{1 - e^{-\kappa}} + e^{-2\kappa} \tag{23}$$

and thus the right hand side of Eq. 21 is smaller than 0.95 for $U > 6$, from which we have

$$0 \leq \delta_n < \frac{\pi}{2} \qquad \text{if} \quad U > 6 \tag{24}$$

Proposition 1

For any $n = 1, 2, \ldots, a$, the correction $\delta_n$ has an asymptotic expansion in powers of $U^{-1}$ of the form

$$\delta_n = 2S \sum_{k=1}^{\infty} c_k U^{-k}$$

$$S = \sin \frac{n\pi}{a+1} \quad , C = \cos \frac{n\pi}{a+1} \tag{25}$$

where, . for $m \geq 3$ :

$$c_1 = 1 \quad , \quad c_2 = -C \frac{a+3}{a+1}$$

. for $m = 2$ :

$$c_1 = 1 \quad , \quad c_2 = -C \frac{a+3}{a+1} + \cos(l\,K)$$

. for $m = 1$

$$c_1 = 1 + \cos(l\,K) \, , \; c_2 = -\frac{2C}{l^2} \left(1 + \cos(l\,K)\right)^2 .$$

In particular, for any width m, the coefficients $c_k$ with $k < m$ are those of the potential well (fig. 5); the first term which depends on m appears at the order $U^{-m}$ in the form $c_m = \tilde{c}_m + \cos(l\,K)$, where $\tilde{c}_m$ is the coefficient for the potential well.

Proof

From Eq. 18 and 19, we have the expansion

$$B = 2U^{-1} + 3E_n U^{-2} + 4(E_n^2 + 1)U^{-3} + O(U^{-4})$$

$$\varepsilon = (1 - e^{-2m\kappa})\, B - e^{-2m\kappa} E_n + O(U^{-2m-2})$$

$$ch\kappa = \frac{1}{2}(U - E_n)$$

$$ch2\kappa = \frac{1}{2}(U - E_n)^2 - 1$$

$$chm\kappa = O(U^m)$$

Therefore from Eq. 21, we have first for any m

$$\lim_{U \to \infty} \sin \delta_n = 0 \qquad \text{i.e. } \delta_n = o\ (U^{-1})$$

Then, for any $m \geq 2$,

$$\lim_{U \to \infty} U \sin \delta_n = 2 \sin\left(\frac{n\pi}{a+1}\right) \qquad \text{i.e. } \delta_n = 2SU^{-1} + o(U^{-1})$$

for any $m \geq 3$,

$$\lim_{U \to \infty} U^2 \left[\sin \delta_n - 2SU^{-1}\right] =$$

$$= \lim_{U \to \infty} U^2 \left[(2U^{-1} + 3E_n U^{-2})\ (S + \frac{a}{a+1} 2SCU^{-1}) - 2SU^{-1}\right] =$$

$$= -2SC\frac{a+3}{a+1} \qquad \text{i.e. } \delta_n = 2SU^{-1} - 2SC\frac{a+3}{a+1}U^{-2} + o(U^{-2})$$

On the other hand, for $m = 2$

$$\lim_{U \to \infty} U^2 \left[\sin \delta_n - 2SU^{-1}\right] = -2SC\frac{a+3}{a+1} + 2S\cos(lK)$$

while for m = 1

$$\lim_{U \to \infty} U \sin \delta_n = 2 S \left(1 + \cos (l K)\right)$$

$$\lim_{U \to \infty} U^2 \left[\sin \delta_n - 2 S (1 + \cos l K) U^{-1}\right]$$

$$= -4 C S \frac{(1 + \cos l K)^2}{(a + 1)^2}$$

Since $\varepsilon(\delta_n)$ (Eq. 19) is of the form

$$\varepsilon (\delta_n) = \sum_{\substack{k \geq 1 \\ r \geq 0}} c_{k,r} U^{-k} \delta_n^r$$

(series which is absolutely convergent for $|U| > 4$) the right hand side of Eq. 21 is of the form

$$\sum_{k \geq 1} U^{-k} \left[ d_k S + \sum_{r \geq 1} d_{k,r} \delta_n^r \right]$$

$$+ \cos (l K) \sum_{k \geq m} U^{-k} \left[ d_k' S + \sum_{r \geq 1} d_{k,r}' \delta_n^r \right]$$

We can thus conclude that $\delta_n$ has the asymptotic expansion stated by Proposition 1.

<u>Proposition 2</u>

For any n = 1, 2, ... , a, the eigenvalue $E_{n,K}$ has the asymptotic expansion

$$E_{n,K} = -2 C - 4 \frac{S^2}{a + 1} \sum_{k \geq 1} d_k U^{-k} \tag{26}$$

$$C = \cos\left(\frac{n \pi}{a + 1}\right) \quad , S = \sin \left(\frac{n \pi}{a + 1}\right)$$

where, . for $m \geq 3$

$$d_1 = 1 \quad , \quad d_2 = -C\,\frac{a+4}{a+1}$$

. for $m = 2$

$$d_1 = 1 \quad , \quad d_2 = -C\,\frac{a+4}{a+1} + \cos(l\,K)$$

. for $m = 1$

$$d_1 = 1 + \cos(l\,K)\,, \quad d_2 = -C\,\frac{3}{a+1}\left(1+\cos(l\,K)\right)^2$$

$$l\,K = \frac{2\pi}{N_o}\,\{1, 2, \ldots, N_o\}. \tag{27}$$

We should again notice that for any m, the coefficients $d_k$ with $k < m$ are those of the potential well (fig. 5), and at the order $U^{-k}$ with $k < m$ the energy level is $N_o$ time degenerate.

Proof : This property is a direct consequence of property 1 and the expansion

$$E_n = -2 \sum_{k \geq 0} \frac{(-1)^k}{(2k)!} \left(\frac{\delta_n}{a+1}\right)^{2k} \left[C + \frac{S}{2\,k+1} \cdot \frac{\delta_n}{a+1}\right] \tag{28}$$

## 3.3. Asymptotic Expansion for the Ground State Energy

We consider the system defined in Sec. 3.1 , with

$$\rho_i = \frac{p}{q}\ , \ l = \nu q\ , \ m = \nu p\ , \ a = \nu(q-p)$$

Proposition 3

For the electron density

$$\rho_e = \frac{\bar{n}}{l}, \quad \bar{n} = 1, 2, \ldots, a \qquad \left(\frac{a}{l} = 1 - \rho_i\right)$$

the ground state energy has the asymptotic expansion :

$$E_N(\rho_e) = E(U = \infty; \rho_e) - \frac{1}{a+1} \sum_{k \geq 1} c_k(\rho_e; \nu) \; U^{-k}$$

where

$$E(U = \infty; \rho_e) = \frac{1}{l}\left[1 - \frac{\sin\left(\frac{\pi}{2} \frac{2 l\rho_e + 1}{a+1}\right)}{\sin\left(\frac{\pi}{2} \frac{1}{a+1}\right)}\right]$$

$$c_1(\rho_e; \nu) = 2\left[\rho_e - \frac{1}{l} \frac{\cos\left(\pi \frac{l\rho_e + 1}{a+1}\right) \sin\left(\pi \frac{l\rho_e}{a+1}\right)}{\sin\left(\pi \frac{1}{a+1}\right)}\right] \tag{29}$$

Moreover, for $\rho_e = 1 - \rho_i$

$$E_N(\rho_e) = -\frac{2}{l} U^{-1} + O(U^{-3}) \tag{30}$$

<u>Proof</u>

For $\bar{n} = l\,\rho_e$, we have $N_e = N_o\, l\, \rho_e = N_o\, \bar{n}$, i.e. all the $\bar{n}$ first "bands" are filled with $N_o$ electrons. Thus

$$E_N(\rho_e) = \frac{1}{l} \sum_{n=1}^{\bar{n}} \frac{1}{N_o} \sum_{\substack{r=1 \\ l K = \frac{2\pi}{N_o} r}}^{N_o} E_{n,K} \tag{31}$$

Using proposition 2, together with the identities

$$2 \sum_{n=1}^{\bar{n}} \cos\left(\frac{n\pi}{a+1}\right) = -1 + \frac{\sin\left(\frac{\pi}{2}\frac{2\bar{n}+1}{a+1}\right)}{\sin\left(\frac{\pi}{2}\frac{1}{a+1}\right)}$$

(32)

$$2 \sum_{n=1}^{\bar{n}} \sin^2\left(\frac{n\pi}{a+1}\right) = \bar{n} - \frac{\cos\left(\pi\frac{\bar{n}+1}{a+1}\right)\sin\left(\pi\frac{\bar{n}}{a+1}\right)}{\sin\left(\pi\frac{1}{a+1}\right)},$$

the first part of the proposition is established. To conclude the second part, we notice first that $E(U = \infty; \rho_e) = 0$ for $\rho_e = 1 - \rho_i$; then computing the coefficient at the order $U^{-2}$ we find $c_2(\rho_e; \nu) = 0$ for $\rho_e = 1 - \rho_i$.

Remarks

1. For any width m, the function $E_N(\rho_e)$ at the order $U^{-k}$, with $k < m$, is linear for $\bar{n}-1 \le \rho_e l \le \bar{n}$ ($E_N(\rho_e) = 0$ for $\rho_e = 0$). Furthermore, at this order, the value of $E_N(\rho_e)$ for $\rho_e l = \bar{n}$, is given by the eigenvalue $E_{\bar{n}}$ of the square well potential (fig. 5). This remark leads us to conjecture that for any periodic configuration of ion, the ground state energy has an expansion

$$E(\rho_e; s) = \sum_{k \ge 0} d_k(\rho_e; s)\, U^{-k}$$

where at the order $k < m$, with m the number of ions in the smallest cluster of ions, the coefficient $d_k$ is obtained using the eigenvalues of the square well potential. In the attractive case, ($U < 0$), we just have to replace "ions" by "holes".

2. For $U = \infty$, we have

$$E_N(U = \infty; \rho_e) = -\frac{2}{\pi}(1 - \rho_i)\sin\left(\pi\frac{\rho_e}{1-\rho_i}\right) + \frac{1}{\nu q}\left[A(\rho_e, \rho_i) + B(\nu; \rho_e, \rho_i)\right] \tag{33}$$

where : $A(\rho_e, \rho_i) + B(\nu; \rho_e, \rho_i) > 0$ for $\rho_e \neq 0$ or $(1 - \rho_i)$

and

$$A(\rho_e, \rho_i) = 1 - \frac{2}{\pi} \sin\left(\pi \frac{\rho_e}{1-\rho_i}\right) - \left(1 - \frac{2\rho_e}{1-\rho_i}\right) \cos\left(\pi \frac{\rho_e}{1-\rho_i}\right) \tag{34}$$

$B = O(\nu^{-1})$.

3. We should note that $c_1(\rho_e ; \nu) > 0$ (Eq. 29) and for $\nu \to \infty$ we have

$$\lim_{\nu \to \infty} c_1(\rho_e) = 2\rho_e \left[1 - \frac{1-\rho_i}{2\pi\rho_e} \sin\left(2\pi \frac{\rho_e}{1-\rho_i}\right)\right] \tag{35}$$

4. Using standard perturbation theory one can show that the asymptotic expansion converges. The question however whether the radius of convergence can be bounded by a constant independent of $\nu$ (or a) remains open.

### 3.4. Bounds on the Ground State Energy

Using Eqs. 22, 19, 18, it is possible to derive upper and lower bounds for $\delta_n$ :

$$\delta_n' \leq \delta_n \leq \delta_n''$$

$$\text{for } m = 1 : \begin{cases} \delta_n' = \frac{2}{U}\left(1 - \frac{c_1'}{U}\right)[1 + \cos(l\,K)]\,S \\ \delta_n'' = \frac{2}{U}\left(1 + \frac{c_1''}{U}\right)[1 + \cos(l\,K)]\,S \end{cases}$$

$$\text{for } m \geq 2 : \begin{cases} \delta_n' = \frac{2}{U}\left(1 - \frac{c'}{U}\right) S \\ \delta_n'' = \frac{2}{U}\left(1 + \frac{c''}{U}\right) S \end{cases}$$

where the constant $c_1'$, $c_1''$, $c'$, $c''$ are independent of (U, a, m) for $U > U_0$. For example, for $U > 8$ we find $c_1' = 4$, $c_1'' = 12$, $c' = 5$, $c'' = 27$.
From the bounds on $\delta_n$, we can then obtain bounds on the energy levels

$$E_n = -2\cos\left(\frac{n\pi - \delta_n}{a+1}\right), \quad C = \cos\left(\frac{n\pi}{a+1}\right), \quad S = \sin\left(\frac{n\pi}{a+1}\right)$$

for m = 1

$$E_n \geq -2C - U^{-1}\frac{4}{a+1}\left(1 + \frac{D_1'}{U}\right)[1 + \cos(l\,K)]\ S^2$$

$$E_n \leq -2C - U^{-1}\frac{4}{a+1}\left(1 - \frac{D_1''}{U}\right)[1 + \cos(l\,K)]\ S^2$$

where $D_1' = 13{,}5$ and $D_1'' = 7$ for $U > 8$,

for $m \geq 2$

$$E_n \geq -2C - U^{-1}\frac{4}{a+1}\left(1 + \frac{D'}{U}\right) S^2$$

$$E_n \leq -2C - U^{-1}\frac{4}{a+1}\left(1 - \frac{D''}{U}\right) S^2$$

where $D' = 37$ and $D'' = 22$ for $U > 8$.

### 3.5. Results

Using the bounds on the energy levels and Eq. 31, we have the following :

Proposition 4

For the ion density $\rho_i = \frac{p}{q}$ and the electron density $\rho_e = \frac{\bar{n}}{l}$, $\bar{n} = 1, 2, \ldots, a$, where $l = \nu q$, $a = \nu q(1 - \rho_i)$, the ground state energy is given by

$$E(U, \rho_e; \rho_i) = -\frac{2}{\pi}(1 - \rho_i) \sin\left(\pi \frac{\rho_e}{1-\rho_i}\right) +$$

$$+ \frac{1}{\nu q}\Big\{A(\rho_e, \rho_i) + B(\nu; \rho_e, \rho_i)$$

$$- \frac{c_1(\rho_e; \nu)}{1-\rho_i + \frac{1}{\nu q}} \left(1 + O(U^{-1})\right) U^{-1}\Big\} \tag{36}$$

where $|O(U^{-1})| < D\, U^{-1}$ with D independent of $(\rho_e, \rho_i, \nu)$ for $U > U_0$ (we have given explicit value for $U_0 = 8$), and $c_1(\rho_e; \nu) > 0$ is defined by Eq. 29.

Theorem

i) For $\rho_e = 1 - \rho_i$ and U sufficiently large the crenel configuration with minimal energy corresponds to $\nu = 1$.

ii) For $\rho_e < 1 - \rho_i$, there exists $U(\rho_e)$ such that for $U > U(\rho_e)$, the segregated configuration ($\nu = \infty$) has minimal energy.

Proof

i) For $\rho_e = 1 - \rho_i$, we have obtained

$$E(U, \rho_e, \rho_i) = -\frac{2}{\nu q} U^{-1} + O(U^{-3})$$

and we have explicit bounds on the rest, which do not depend on $\nu$. Therefore, if U is sufficiently large, the configuration with $\nu = 1$ will have minimal energy.

ii) For $\rho_e < 1 - \rho_i$, the coefficient of $\nu^{-1}$ in Eq. 36 is positive for U sufficiently large and thus the energy decreases as $\nu \to \infty$. In fact, for $\nu \to \infty$, it follows from Eq. 34 and 35 that the coefficient of $\nu^{-1}$ in Eq. 36 is :

$$\{\cdots\} = 1 - \frac{2}{\pi} \sin\left(\pi \frac{\rho_e}{1-\rho_i}\right) - \left(1 - \frac{2\rho_e}{1-\rho_i}\right) \cos\left(\pi \frac{\rho_e}{1-\rho_i}\right)$$

$$- \frac{1}{\pi}\left(\frac{2\pi\rho_e}{1-\rho_i} - \sin\left(2\pi \frac{\rho_e}{1-\rho_i}\right)\right) \left(1 + O\left(U^{-1}\right)\right) U^{-1}$$

This last expression indicates that the value U ($\rho_e$), at which the segregated phase appears, is an increasing function of $\rho_e$ (Figs. 6,7).

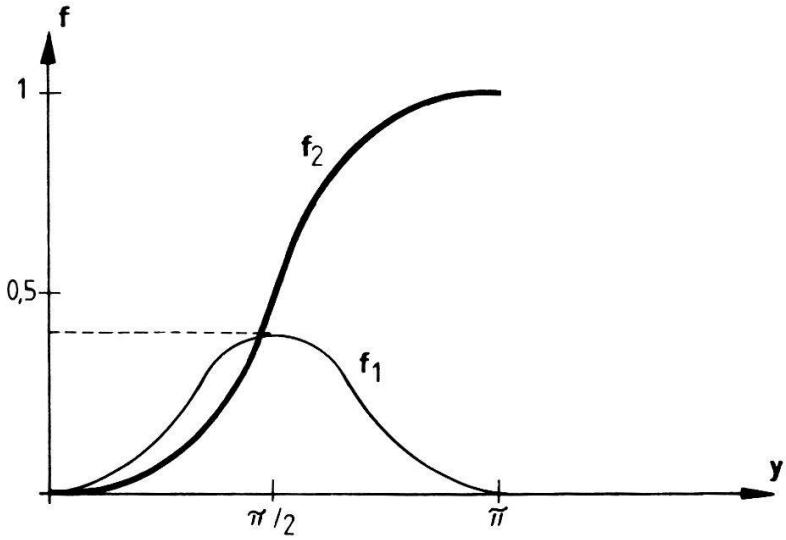


Fig. 6 : $f_1(y) = 1 - \frac{2}{\pi} \sin y - \left(1 - \frac{2y}{\pi}\right) \cos y$

$f_2(y) = \frac{1}{2\pi}\left(2y - \sin(2y)\right)$

$\overline{y} = \pi \frac{\rho_e}{1-\rho_i}$

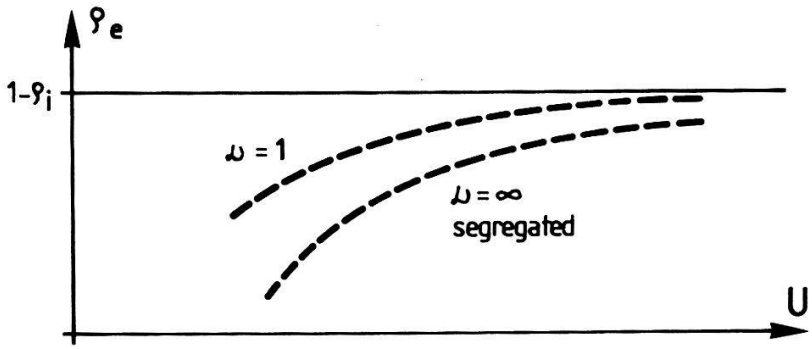


Fig. 7 : Phase diagram for the crenel configurations with $\rho_i = \frac{p}{q}$

Corollary

For any ion density $\rho_i = \frac{p}{q}$ there exists $\rho_e' = \rho_e'(U; q)$ and $\rho_e'' = \rho_e''(U; q)$ such that for $\rho_e < \rho_e'$, the configuration with $\nu = \infty$ (= segregated configuration) has minimum energy, while for $\rho_e > \rho_e''$ it is the configuration with $\nu = 1$ (fig. 7).

This corollary is a direct consequence of the theorem together with the convexity property of $E(\rho_e)$.

Remark

We have established Proposition 4 only for discrete values of the electron density, i.e. $\rho_e = \frac{\bar{n}}{\nu q}$ $\left(\text{recall that } \rho_i = \frac{p}{q}\right)$. However, the two main points of the proofs are the existence of uniform bounds, and the fact that :

$$E(U; \rho_e, \rho_i) = E_{seg}(\rho_e, \rho_i) + \frac{1}{\nu q}[\alpha - \beta U^{-1}]$$

where $\alpha$ and $\beta$ have a limit as $\nu \to \infty$ with $\alpha > 0$ if $\rho_e < 1-\rho_i$ and $\alpha = 0$ if $\rho_e = 1-\rho_i$.

In other words, the increase of kinetic energy and the decrease of potential energy are both proportionals to $\nu^{-1}$. These two points will remain valid for $\bar{n}\, l < \rho_e < (\bar{n} + 1)\, l$.

## 4. Concluding remarks

We have shown that the crenel configuration with minimal energy is given by the periodic configuration with period q $\left(\rho_i = \frac{p}{q}\right)$ if the electron density $\rho_e$ is such that $\rho_e'' \leq \rho_e \leq 1-\rho_i$ (or $\rho_e'' \leq \rho_e \leq \rho_i$ in the attractive case $U < 0$); on the other hand if $\rho_e < \rho_e'$ it is the segregated configuration.

However, it should be stressed that we do not infer that the crenel configuration with period q is a ground state (with respect to all possible configurations). Such a statement is in fact wrong for ion densities $\rho_i = \frac{p}{q}$ with $2 \leq p \leq q-1$; indeed in such cases we can always consider the mixture of the

configuration $\rho_i = \frac{1}{2}$ with period 2, and the configuration $\rho_i = 0$ (if $2p \leq q$) or $\rho_i = 1$ (if $2p \geq q$), i.e.

$$\text{if } 2p \leq q : \quad s = 2\,\frac{p}{q}\,\rho_i\,[\tfrac{1}{2}] + \frac{q-2p}{q}\,\rho_i\,[0]$$

$$\text{if } 2p \geq q : \quad s = 2\,\frac{(q-p)}{q}\,\rho_i\,[\tfrac{1}{2}] + \frac{2p-q}{q}\,\rho_i\,[0]$$

From Eq. 30, we have :

$$\text{if } 2p \leq q : \quad E(\rho_e; s) = -\frac{2p}{q}\,U^{-1} + O(U^{-3})$$

$$\text{if } 2p \geq q : \quad E(\rho_e; s) = -\frac{q-p}{q}\,U^{-1} + O(U^{-3})$$

On the other hand, for the periodic configuration with period q

$$E(\rho_e) = -\frac{2}{q}\,U^{-1} + O(U^{-3})$$

Using the explicit bounds we have obtained, we can find $U_o$ such that for $U > U_o$ the mixture configuration has energy smaller than the periodic one. Therefore for ion densities $\rho_i = p/q$, with $p \neq 1$ or q, the crenel configuration with period q is not a ground state configuration for $\rho_e = 1-\rho_i$ (or $\rho_e = \rho_i$ if $U < 0$).

What is the situation for $\rho_i = \frac{1}{q}$ and $\rho_i = 1 - \frac{1}{q}$ ? We shall discuss only the case $\rho_i = 1 - \frac{1}{q}$ (i.e. $\rho_i = \frac{1}{q}$ for the attractive interaction $U < 0$). In this case $a = \nu$, and thus, for the periodic configuration with period q (i.e. $\nu = 1$), we obtain from proposition 2 with $n = a = 1$, $\cos(l\,K) = -1$ :

$$E_{1,K} = -2\,U^{-1} + O(U^{-3}) \qquad \text{if } q > 2$$

$$E_{1,K} = 0 \qquad \text{if } q = 2$$

It follows that the tangent of the function $E(\rho_e)$ at $\rho_e = 1 - \rho_i$ will intersect $E_{seg}(\rho_e)$ if

$$E(\rho_e = 1 - \rho_i) > -\frac{2}{\pi}\,(1-\rho_i)\,.$$

But we have seen that

$$E(\rho_e = 1 - \rho_i) > -\frac{2}{q}\left(1 + \frac{37}{U}\right) U^{-1}$$

Therefore, at least, for $U > 12$, we can conclude that the convex envelope of the functions $E_{seg}(\rho_e)$ and $E(\rho_e; s)$, with s the periodic configuration with period q, coincides with $E(\rho_e; s)$ only at $\rho_e = 1-\rho_i \left(=\frac{1}{q}\right)$.

Proposition 5

For $\rho_i = 1 - \frac{1}{q}\left(\text{or } \rho_i = \frac{1}{q} \text{ if } U < 0\right)$ the periodic configuration with period q can be a ground state configuration only for $\rho_e = 1 - \rho_i$ (or $\rho_e = \rho_i$ if $U < 0$). Furthermore, there exists $\rho_e^c = \rho_e^c(U)$ such that for $\rho_e^c < \rho_e < 1 - \rho_i$, the mixture of the segregated and the periodic configuration with period q, has energy smaller than the other two configurations; for $\rho_e < \rho_e^c$ the segregated configuration has energy smaller than the periodic and the mixture.

The last question which remains open is thus to prove that the crenel configuration with period q is the true ground state with respect to all configurations. To illustrate this point, let us consider the densities $\rho_i = \frac{2}{3}$ and $\rho_i = \frac{3}{4}$ $(U > 0)$. Taking mixtures consisting of the configurations $\rho_i = \frac{1}{2}$ and $\rho_i = 0$, we notice that, at the order $U^{-1}$, the periodic configuration and the mixture have the same energy. However, as it is shown in the Appendix, at the order $U^{-2}$ the periodic configurations have energy smaller than the mixture. In the case $\rho_i = \frac{1}{4}$, we could then consider a mixture of $\rho_i = \frac{1}{3}$ and $\rho_i = 0$; going to the order $U^{-3}$ we see again that the periodic configuration has energy smaller than the mixture. We are thus led to conjecture that for $\rho_i = 1 - \frac{1}{q}\left(\text{or } \rho_i = \frac{1}{q} \text{ if } U < 0\right)$ the periodic configuration with period q is the true ground state.

Acknowledgments

It is a pleasure to thank A. Sütö for many useful discussions.

## Appendix

The case $\rho_i = \frac{q-1}{q}$ , $\rho_e = \frac{1}{q}$ is particularly simple since it corresponds to $a = 1$ and thus $n = a = 1$ in Eq. 21 (for the attractive potential $U < 0$ it corresponds to $\rho_i = \rho_e = \frac{1}{q}$).

- For $\rho_i = \frac{1}{2}$, the energy spectrum is known exactly and for the levels in [-2, +2] we have :

$$E = \frac{U}{2} - \sqrt{\left(\frac{U}{2}\right)^2 + (2 \cos K)^2} \qquad K = \frac{\pi}{N_o} \{1, 2, \dots, N_o\}$$

which gives the expansion

$$E = -2\,(1 + \cos 2\,K)\,U^{-1} + 4\,(1 + \cos 2\,K)^2\,U^{-3} + O\,(U^{-5}) \tag{A.1}$$

and for the ground state energy

$$E_F\left(\rho_e = \frac{1}{2}; \rho_i = \frac{1}{2}\right) = -U^{-1} + 3\,U^{-3} + O\,(U^{-5}) \tag{A.2}$$

- For arbitrary $q \geq 3$ , $\rho_i = \frac{q-1}{q}$ ,

$$E = -2 \sin\left(\frac{\delta}{2}\right)$$

and Eq. 21 yields, with $m = q - 1 \geq 2$,

$$E = -\varepsilon - \cos(q\,K)\,\left[\mathrm{ch}\,(m\,\kappa)\right]^{-1} \tag{A.3}$$

with

$$\varepsilon = 2\,U^{-1} + 3\,E\,U^{-2} + 4\,(1 + E^2)\,U^{-3} + 15\,E\,U^{-4}$$

$$+ 12\,U^{-5} - E\,U^{-2m} - 4\,U^{-2m-1} + O\,(U^{-6}) \tag{A.4}$$

$$\left[\mathrm{ch}\,(m\,\kappa)\right]^{-1} = 2\,U^{-m}\,(1 + m\,E\,U^{-1} + m\,U^{-2}) \;+\; O\,(U^{-6})$$

At the order $U^{-3}$ we thus have for the energy levels

$$E \;=\; -2\,U^{-1} \;+\; 2\;U^{-3} - 2\cos\,(qK)\;\left[U^{-2}\,\delta_{q;3} \;+\; U^{-3}\;\delta_{q;4}\right]$$

(where $\delta_{q;n}$ is the Kronecker symbol)

and for the ground state energy

$$E_F\left(\rho_e = \frac{1}{q}\right) = \frac{2}{q}\;\left[-\,U^{-1} \;+\; U^{-3} \;+\; O\,(U^{-5})\right] \tag{A.5}$$

Therefore the ground state energy per unit period (i.e. $q\;E_F$) for $q \geq 3$ is smaller than for $q = 2$, (for large U).

At the order $U^{-5}$ , we find :

. for $q = 3$

$$E \;=\; -2\;U^{-1} \;+\; 2\,U^{-3} - 2\,U^{-5}$$

$$-\,2\cos\,(qK)\;\left[U^{-2} \;-\; 5\,U^{-4} \;-\; 4\;\cos\,(qK)\;U^{-5}\right]$$

$$E_F\left(\rho_e = \frac{1}{q}\right) = \frac{2}{q}\;\left[-\,U^{-1} \;+\; U^{-3} \;-\; U^{-5} \;+\; O\,(U^{-7})\right] \tag{A.6}$$

. for $q = 4$

$$E \;=\; -2\,U^{-1} \;+\; 2\;U^{-3} - 4\,U^{-5} - 2\cos\,(qK)\;\left[U^{-3} - 6\;U^{-5}\right]$$

$$E_F\left(\rho_e = \frac{1}{q}\right) = \frac{2}{q}\;\left[-\,U^{-1} \;+\; U^{-3} \;-\; 2\;U^{-5} \;+\; O\,(U^{-7})\right] \tag{A.7}$$

. for $q \geq 5$

$$E = -2\,U^{-1} + 2\,U^{-3} - 4\,U^{-5} - 2\cos(qK)\left[U^{-4}\,\delta_{q;4} + U^{-5}\,\delta_{q;5}\right]$$

$$E_F\left(\rho_e = \frac{1}{q}\right) = \frac{2}{q}\left[-U^{-1} + U^{-3} - 2\,U^{-5} + O\left(U^{-7}\right)\right] \tag{A.8}$$

Therefore the ground state energy per unit period for $q \geq 4$ (Eqs. A.7 and A.8) is smaller than for $q = 3$ and $q = 2$ (Eqs. A.6, A.5).

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