

Ground states of continuum models

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Abstract

We calculate the ground state energies of a system of electrons in one-dimensional infinitely deep square well potentials. We analyze the cases when the wells are regularly spaced and when they are clustered together to form one single large well. These potentials are intended to physically describe the interaction of electrons and nuclei in a continuum model. We investigate which potential yields the minimum ground state energy using elements of interpolation potential in quantum mechanics derived from first principles. We also mention models of crystalline formation that are related to this problem.

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We calculate the ground state energies of a system of electrons in one-dimensional infinitely deep square well potentials. We analyze the cases when the wells are regularly spaced and when they are clustered together to form one single large well. These potentials are intended to physically describe the interaction of electrons and nuclei in a continuum model. We investigate which potential yields the minimum ground state energy using elements of interpolation potential in quantum mechanics derived from first principles. We also mention models of crystalline formation that are related to this problem.

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I. INTRODUCTION

We study a system of electrons in infinitely deep square well potentials in two situations. In the first situation the potential consists of M regularly spaced wells, each of them having the form

$$V_r(x) = \begin{cases} 0 & \text{for } (j-1)(b+a) \leq x \leq j(b+a) - a \\ \infty & \text{for } x = (j-1)(b+a) \text{ and } x = j(b+a) - a \end{cases} \quad (1)$$

for $j = 1, 2, 3, \dots, M$.

In the second situation, the M wells are all clustered together forming one single large well. The corresponding potential is

$$V_c(x) = \begin{cases} 0 & \text{for } 0 < x < M(b+a) - a \\ \infty & \text{for } x = 0 \text{ and } x = M(b+a) - a. \end{cases} \quad (2)$$

The potential (1) is intended to represent electrons bound to individual nuclei arranged in an orderly pattern whereas potential (2) is intended to represent electrons bound to the set of nuclei.

We are interested in the ground state of a system of N electrons in potentials (1) and (2), and we would like

to compare the ground state energies in these potentials in order to determine whether the lowest ground state energy corresponds to the configuration of potential (1) or of potential (2). The ordered arrangement of potential (1) is interpreted as corresponding to crystallization or existence of a periodic ground state.

This is a very simplified version of a much broader problem of understanding crystallization in continuum models and of determining whether crystallization is in any way induced by the discrete character of the lattice models in which this phenomenon has been observed^{1,2}. At low temperatures, matter displays a crystalline structure. The particles of matter are arranged in an orderly pattern that is repeated throughout the material. This arrangement is associated with a minimum energy of the system.

One of the lattice models of crystalline formation is the Falicov-Kimball model. This is a lattice model in which ions are fixed at the lattice sites and spinless electrons move about and interact with the ions only when they both happen to occupy the same site. There is no interaction between electrons. For certain values of the ion-electron interaction and for certain values of the number of particles present, the ions display a checkerboard pattern in the ground state of the model. This regular configuration of the ions is associated with the existence of periodic ground states. See³ for details and further results on this model.

In the present case, the question is immediately raised whether it is legitimate to compare ground state energies for two *different* potentials. It is clear that if we consider two energy states for the **same** potential then the state with lower energy is the ground state. We show that the comparison of ground state energies in this case is meaningful. The key ingredient is a varying parameter that will provide a transition from potential (2) to that of Eq. (1) thus allowing for the comparison of ground state energies. This is carried out in section II.

Next in section III we find that the ground state energy for potential (1) is always **higher** than that for potential (2) and hence the minimum ground state energy does not correspond to the arrangement of electrons in potential (1).

II. THE INTERPOLATION POTENTIAL

The comparison of energies for the different potentials of Eqs. (1) and (2) is meaningful because the potential V_h shown in Fig. 1 interpolates between these two cases, with $h \rightarrow \infty$ being potential (1) and $h \rightarrow 0$ being potential (2).

For electrons on an interval $[p, q]$, let $\mathcal{H}_{[p,q]}$ be the Hilbert space of single-electron states. For **spinless** electrons, $\mathcal{H}_{[p,q]} = L^2([p, q], dx)$. It follows that for finite h single-electron states under the potential of Fig. 1 lie on $\mathcal{H}_{[0,2b+a]} = L^2([0, 2b + a], dx)$, and a vector state of a system of N electrons will lie on the closed

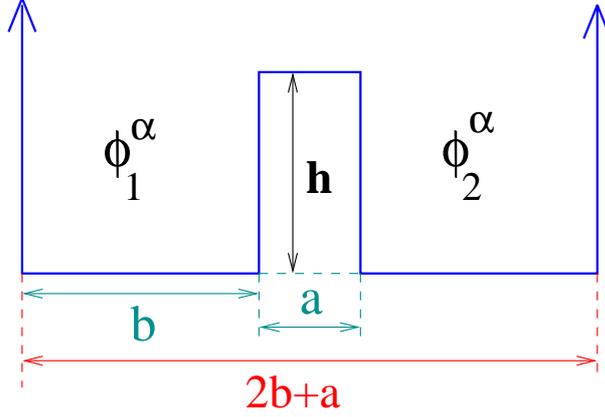


FIG. 1: This potential interpolates between potentials of Eqs. (1) and (2) when $M = 2$ as the height h is sent to infinity or zero respectively.

antisymmetric subspace $\mathcal{H}_{[0,2b+a]}^N$ of

$$\mathcal{H}_{[0,2b+a]}^N = \underbrace{\mathcal{H}_{[0,2b+a]} \otimes \cdots \otimes \mathcal{H}_{[0,2b+a]}}_{N \text{ times}}.$$

For N normalized single-electron states $\Psi_h^{\alpha\nu} \in \mathcal{H}_{[0,2b+a]}$ for $\nu = 1, 2, \dots, N$ the anti-symmetrization operator \mathcal{A} is given by

$$\mathcal{A}(\Psi_h^{\alpha_1} \otimes \cdots \otimes \Psi_h^{\alpha_N}) = \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} \epsilon_\pi \Psi_h^{\alpha_{\pi(1)}} \otimes \cdots \otimes \Psi_h^{\alpha_{\pi(N)}}, \quad (3)$$

where S_N is the permutation group of N elements and ϵ_π equals ± 1 according to the parity of π . In coordinate space the wave-function for a system of N electrons is given by the well-known Slater determinant

$$\Psi_h^\alpha(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} \epsilon_\pi \Psi_h^{\alpha_{\pi(1)}}(x_1) \otimes \cdots \otimes \Psi_h^{\alpha_{\pi(N)}}(x_N). \quad (4)$$

If H_h^N is the Hamiltonian of N non-interacting electrons under the potential of Fig. 1, then H_h^N acts in the antisymmetric subspace $\mathcal{H}_{[0,2b+a]}^N$ as

$$H_h^N = \sum_{\nu=1}^N \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{\nu-1 \text{ times}} \otimes H_h \otimes \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{N-\nu \text{ times}},$$

where H_h is the single-electron Hamiltonian (without spin interactions)

$$H_h = -\frac{\hbar^2}{2\mu} \nabla^2 + V_h, \quad (5)$$

acting on $\mathcal{H}_{[0,2b+a]}$, with μ being the mass of the electron.

What happens now when the limit $h \rightarrow \infty$ is taken? If $\Psi_h^\alpha \in \mathcal{H}_{[0, 2b+a]}$ is a normalized wave-function of a single electron under the potential V_h of Fig. 1 then, when $h \rightarrow \infty$, due to exponential damping of Ψ_h^α on the interval $[b, b+a]$, one has

$$\Psi_h^\alpha \xrightarrow{h \rightarrow \infty} c_1 \phi_1^\alpha + c_2 \phi_2^\alpha \quad (6)$$

where ϕ_i^α for $i = 1, 2$ are the normalized wave-functions defined in each of the potential wells obtained from Fig. 1 after h goes to infinity.

According to our notation ϕ_1^α lies on $\mathcal{H}_{[0, b]}$ and ϕ_2^α lies on $\mathcal{H}_{[b+a, 2b+a]}$. Due to the normalization condition in (6), the coefficients satisfy $|c_1^\alpha|^2 + |c_2^\alpha|^2 = 1$. According to our notation, ϕ_1^α lies on $\mathcal{H}_{[0, b]}$ and ϕ_2^α lies on $\mathcal{H}_{[b, 2b+a]}$. Both $\mathcal{H}_{[0, b]}$ and $\mathcal{H}_{[b, 2b+a]}$ are closed orthogonal subspaces of $\mathcal{H}_{[0, 2b+a]}$ and the sums in (6) can be interpreted as direct sums.

On the other hand, the single-electron Hamiltonian H_h in (5) converges, in the limit $h \rightarrow \infty$, to a direct sum $\mathcal{H}_h = H_1 + H_2$ acting on $\mathcal{H}_{[0, b]} \oplus \mathcal{H}_{[b, 2b+a]}$, where H_1 and H_2 are the single-electron Hamiltonians $-\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2}$ restricted, respectively, to the intervals $[0, b]$ and $[b, 2b+a]$.

The crucial observation to make is that if Ψ_h^α are normalized eigenstates of H_h , i.e. $H_h \Psi_h^\alpha = E_h^\alpha \Psi_h^\alpha$, then it is not necessarily true that the states ϕ_i^α in (6) are eigenstates of H_i . However, due to the exponential damping of Ψ_h^α on the interval $[b, b+a]$ that, in the limit $h \rightarrow \infty$,

$$E_h^\alpha = (\Psi_h^\alpha, H_h \Psi_h^\alpha) \rightarrow |c_1^\alpha|^2 (\phi_1^\alpha H_1 \phi_1^\alpha) + |c_2^\alpha|^2 (\phi_2^\alpha H_2 \phi_2^\alpha), \quad (7)$$

where the right-hand side above is a convex linear combination of the expectation values $(\phi_1^\alpha H_1 \phi_1^\alpha)$ and $(\phi_2^\alpha H_2 \phi_2^\alpha)$.

It now follows that in the resulting symmetric potential of Fig. 1 obtained after taking the limit $h \rightarrow \infty$ we have $E_1^\alpha = (\phi_1^\alpha H_1 \phi_1^\alpha) = E_2^\alpha = (\phi_2^\alpha H_2 \phi_2^\alpha) = E^\alpha$, so that

$$E_h^\alpha = (\Psi_h^\alpha, H_h \Psi_h^\alpha) \rightarrow (\phi_i^\alpha H_i \phi_i^\alpha) = E^\alpha. \quad (8)$$

For the case of multi-particle states $\mathcal{A}(\Psi_h^{\alpha_1} \otimes \dots \otimes \Psi_h^{\alpha_N})$, with $\Psi_h^{\alpha_\nu}$ being eigenstates of H_h , the total energy is $\sum_{\nu=1}^N E_h^{\alpha_\nu}$. In this case, (7) now converges, as $h \rightarrow \infty$, to

$$\sum_{\nu=1}^N E_h^{\alpha_\nu} \rightarrow \sum_{\nu=1}^N \left[|c_1^{\alpha_\nu}|^2 (\phi_1^{\alpha_\nu}, H_1 \phi_1^{\alpha_\nu}) + |c_2^{\alpha_\nu}|^2 (\phi_2^{\alpha_\nu}, H_2 \phi_2^{\alpha_\nu}) \right].$$

The same observations made above about ϕ_i^α being eigenstates and the fact that the resulting potentials are symmetric now lead, when $h \rightarrow \infty$, to

$$E_h^\alpha = \sum_{\nu=1}^N E_h^{\alpha_\nu} \rightarrow \sum_{\nu=1}^N (\phi_1^{\alpha_\nu}, H_1 \phi_1^{\alpha_\nu}) = \sum_{\nu=1}^N E^{\alpha_\nu}. \quad (9)$$

The results (8) and (9) allow us to obtain a **lower** bound to E_h^α by taking respectively the minimum value of E^α and $E^{\alpha\nu}$ in these expressions. The important point is that the minimum value of the right-hand side of (9) is exactly the energy of the system of electrons which is obtained by successively filling up the single-electron energy levels of potential of Eq. (1) from the lowest levels up in each infinite well (Section III).

This lower bound to the energy of the system of electrons for the potential of Eq. (1) will be compared with an **upper** bound to the energy of the system of electrons for the potential of Eq. (2) (the case $h = 0$) to show that the energy of the electrons is minimized for the potential V_c . Since the parameter h provides a smooth transition from the potential of Eq. (1) to the potential of Eq. (2) when it varies from zero to infinity, we are justified in comparing system energies in the two different potentials.

III. THE GROUND STATE ENERGIES

The corresponding single-electron energies for the potential Eq. (1) are given by⁴

$$e_r = \left(\frac{\pi}{kb}\right)^2 q^2 \quad (10)$$

for $q = 1, 2, 3, \dots$, where b is the length of each well, $k^2 = 2\mu/\hbar^2$, and μ is the mass of the electrons. The ground state energy of a system of N electrons in potential (1) is the sum of the lowest energies in Eq. (10) in each well. In this case, it is convenient to write the total number of electrons as $N = nM + m$ for integers n and m , where m ($m < M$) is the remaining number of electrons after each of the M wells have been filled with n electrons.

The ground state energy is then

$$E_r = \left(\frac{\pi}{kb}\right)^2 \left[M \left(\frac{n^3}{3} + \frac{n^2}{2} + \frac{n}{6} \right) + m(n+1)^2 \right]. \quad (11)$$

Eq. (11) says that after n electrons have been distributed in the M wells, each of the remaining m electrons will be placed on the next higher energy level.

The single-electron energies for the potential of Eq. (2) admit upper bounds given by

$$e_c = \left(\frac{\pi}{Mkb}\right)^2 q^2 \quad (12)$$

for $q = 1, 2, 3, \dots$

The ground state energy of a system of N electrons is again the sum of the successive lowest energies in

Eq. (12). We obtain

$$E_c = \sum e_c = \left(\frac{\pi}{Mkb}\right)^2 \left(\frac{N^3}{3} + \frac{N^2}{2} + \frac{N}{6}\right). \quad (13)$$

By substituting $N = nM + m$ into the above equation, we write

$$E_c = \left(\frac{\pi}{kb}\right)^2 \left\{ \frac{M}{3}n^3 + \frac{2m+1}{2}n^2 + \frac{1+6m+6m^2}{6M}n + \frac{m+3m^2+2m^3}{6M^2} \right\}.$$

To compare the ground state energies, we calculate $\Delta E = E_r - E_c$ and obtain

$$\begin{aligned} \Delta E &= \left(\frac{\pi}{kb}\right)^2 \left[M\left(\frac{n^3}{3} + \frac{n^2}{2} + \frac{n}{6}\right) + m(n+1)^2 \right] - \left(\frac{\pi}{Mkb}\right)^2 \left(\frac{N^3}{3} + \frac{N^2}{2} + \frac{N}{6}\right) \\ &= \left(\frac{\pi}{kb}\right)^2 (xn^2 + yn + z), \end{aligned} \quad (14)$$

where

$$x = \frac{1}{2}(M-1)$$

is always positive for $M > 1$,

$$y = \frac{M}{6} + 2m - \frac{m^2}{M} - \frac{m}{M} - \frac{1}{6M} = \frac{M^2 + 6m(M-1) + 6m(M-m) - 1}{6M} > 0$$

under the conditions $M > 1$ and $m < M$, and

$$z = m - \frac{m+3m^2+2m^3}{6M^2} = \frac{6mM^2 - (2m^3 + 3m^2 + m)}{6M^2} > \frac{m(M^2 - m^2)}{M^2} > 0$$

for $M > 1$ and $m < M$.

We thus conclude that ΔE in Eq. (14) is a positive quantity and the energy of the system for Eq. (2) is always lower than for Eq. (1) for all values of the parameters n , M and m under the given conditions of the problem.

The potentials studied here are of course too simple to answer the fundamental question of crystallization in continuum models. Important interactions have been left out (this is also true of more elaborate models as the Falicov-Kimball model). But they do allow for a definite answer to the problem posed within the simplified assumptions made.

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