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On the Ionization of Crystals

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Abstract. We provide a lower bound for the energy required to ionize an "electron" from a finite crystal of low density and we show that the bound is independent of the crystal size. The electrons interact with each other and with the fixed positive charges by short range interactions from a suitable class of potentials.

I. Introduction

In this article, we prove the following assertion; let $H_M(N, a, m)$ be the Schrödinger operator for M spinless "electrons" of mass m in the presence of N fixed "protons" regularly arranged in a finite lattice with lattice constant a. Assume that the electrons are either Bosons or Fermions and assume that they interact with one another by a positive, short range continuously differentiable potential $v_R(\boldsymbol{x}_i - \boldsymbol{x}_j)$ and interact with the protons by $-v_A(\boldsymbol{x}_i - \boldsymbol{y}_j)$. Here, $\boldsymbol{x}_i$ is the position of the i-th electron and $\boldsymbol{y}_j$ is the position of the j-th proton. Then $H_M(N, a, m)$ has a ground state eigenvalue λ_{MN} uniformly isolated from the continuous spectrum for all N and $M \leqq N$ if a and m are sufficiently large. Hence there is a $g > 0$ such that for all N and $M \leqq N$, dist $(\lambda_{MN}, \sigma_{MN}) \geqq g$ where σ_{MN} is the continuous spectrum of $H_M(N, a, m)$.

The quantity g is a lower bound for the work function familiar from the photoelectric effect, i.e. the amount of energy required to ionize an electron from the crystal. The fact that the work function is non-vanishing insures that the electrons do not spontaneously escape from the crystal, regardless of the crystal size. Thus the result is related to the more general problem concerning the stability of solids.

Let us now outline the strategy of the proof. By Hunziker's theorem [1, 2], the infimum of the essential spectrum for $H_M(N, a, m)$ lies at $\inf_{M' < M}$ {inf spectrum $H_{M'}(N, a, m)$}. We make the inductive hypothesis that this infimum is actually $\lambda_{M-1,N}$ i.e. the ground state for the Hamiltonian with one less electron. It is therefore natural to consider the tensor product of the corresponding ground state eigenfunction $\psi_{M-1,N}$ (not necessarily unique) with a one particle trial function ϕ and to try to show that the energy expectation value for the tensor product is bounded above by $\lambda_{M-1,N} - g$. This would establish the existence of discrete spectrum for $H_M(N, a, m)$ below $\lambda_{M-1,N} - g$ and therefore the existence of a ground state eigenfunction ψ_{MN} corresponding to $\lambda_{MN} =$ inf spectrum $H_M(N, a, m)$. The induction then proceeds to $M \leqq N$. However, there are two modifications to this strategy.

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