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Localised Solutions of Hartree Equations for Narrow-Band Crystals

Claudio Albanese*

Theoretical Physics, ETH-Hönggerberg, CH-8093 Zürich, Switzerland

Abstract. We consider the Hartree equations for a system of an infinite number of electrons in a periodic potential consisting of a periodic array of wells. The filling fraction is assumed to be of one electron per well. We prove that if the wells are deep enough to admit a bound state and if they are separated by a distance large enough, then the Hartree equations have a solution in which all single particle wave functions decay exponentially.

1. Introduction

This note is dedicated to the study of the following eigenvalue problem

$$\begin{cases} -\Delta u + Vu + W(u)u = Eu \\ u \in W^{2,2}(\mathbb{R}^3),\ \|u\|_2 = 1,\ u(x) > 0, \end{cases} \tag{1.1}$$

where

$$V(x) = \sum_{\underline{i} \in \mathbb{Z}^3} U_a(x + \underline{i}l) \tag{1.2}$$

and $W(u)$ is the operator of multiplication times

$$\sum_{\underline{i} \in \mathbb{Z}^3 \setminus \{0\}} \int dy\, W(|y-x|)\, u(y + \underline{i}l)^2 . \tag{1.3}$$

Here l and a are positive parameters such that $l > 2a + \varepsilon$ for some fixed constant $\varepsilon > 0$, $U_a(x)$ is the potential well

$$U_a(x) = \begin{cases} -U & \text{if} \quad |x| \leqq a \\ 0 & \text{if} \quad |x| > a \end{cases}, \tag{1.4}$$

and $W(s)$ is a monotonously decreasing, nonzero function in $L^\infty(\mathbb{R}_+)$, such that

$$0 \leqq W(s) \leqq C_0 s^{-3-\eta} \quad \forall s \geqq 0 \tag{1.5}$$

for some constants $C_0, \eta > 0$.

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* Address after July, 1988: Department of Mathematics, University of California, Los Angeles, CA 90024, USA