

A MODEL BASED UPON THE CROSS-CORRELATION FUNCTION BETWEEN THE POTENTIAL AND WAVE FUNCTIONS FOR DISORDERED SOLIDS

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A formulation for the cross-correlation function between the potential and Schrödinger wave functions with respect to the spacing between consecutive atoms in an infinite one-dimensional disordered solid is proposed. In this theoretical model, the argument of the above cross-correlation function is the spacing in question which is regarded as a random variable.

Keywords: Cross-correlation function; Schrödinger wave functions; disordered solids

1. INTRODUCTION

It is well-known that a solid in crystalline state presents a constant spacing between adjacent atoms; this spacing is the period of the corresponding crystalline lattice. On the other hand, it is also well-known that a given electron in the solid is submitted to a periodic field whose potential energy function is a periodic function whose period coincides with the above spacing. If we consider this spacing as a random variable, we are considering implicitly the solid as a disordered system. In addition, we can claim that a measure of this randomness is a certain correlation function. For clear reasons which will be given later, we shall choose as this function the cross-

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correlation function between the potential function and a generic wavefunction obeying the non-relativistic time-independent Schrödinger equation. Our model deals with one-dimensional disordered solids.

2. THEORY

First of all, let us consider the non-relativistic time-independent Schrödinger equation in one dimension, namely:

$$\frac{d^2}{dx^2}(\psi(x)) + 2m\hbar^{-2}[E - V(x)]\psi(x) = 0 \quad (1)$$

From now on we shall assume an infinite and one-dimensional disordered solid so that from Eq. (1) and considering that $V(x) = V(x + s)$ (V denotes potential energy and s is lattice period), we get:

$$\frac{d^2}{dx^2}(\psi(x + s)) + 2m\hbar^{-2}[E - V(x)]\psi(x + s) = 0 \quad (2)$$

since $\psi(x + s)$ obeys Eq. (1) (we assume real $\psi(x)$).

From expression (2), it follows:

$$\begin{aligned} \xi(s) \equiv \int_0^\infty V(x)\psi(x + s)dx &= \frac{\hbar^2}{2m} \left[\frac{d}{dx}(\psi(x)) \Big|_{x \rightarrow \infty} - \frac{d}{ds}(\psi(s)) \right] \\ &+ E \int_s^\infty \psi(x)dx \end{aligned} \quad (3)$$

where $\xi(s)$ is the cross-correlation function between V and ψ .

Observing relationship (3), we see that the existence of $\xi(s)$ is assured if the Schrödinger eigenfunctions are integrable. Even this condition does not arise from the well-known square-integrability of $\psi(x)$, in practice, the major part of the typical cases in solid state physics (in particular, physics of semiconductors) exhibit the integrability of $\psi(x)$. On the other hand, at this point we want to emphasize that we have assumed $\psi(x)$ as real functions which constitutes a typical situation in practice.

Now, from Eq. (3) it follows:

$$\frac{d}{ds}(\xi(s)) = -E\psi(s) - \frac{\hbar^2}{2m} \frac{d^2}{ds^2}(\psi(s)) \quad (4)$$

In addition, by taking into account expression (3), the expected value of ξ (or average value) is: $\bar{\xi} = \int_0^\infty \xi(s) \chi(s) ds$ so that

$$\bar{\xi} = \frac{\hbar^2}{2m} \left[\frac{d}{dx}(\psi(x)) \Big|_{x \rightarrow \infty} - \overline{\frac{d}{ds}(\psi(s))} \right] + E \int_{s_1}^{s_2} \chi(s) ds \int_s^\infty \psi(x) dx \quad (5)$$

where $\chi(s)$ is the probability density function of $s(s_1 \leq s \leq s_2)$.

Finally, we can establish the following reasonable statement: the expected value of s should coincide with the period of the crystalline counterpart (this period is, of course, fixed); let us denote this period by d . Then, we can write:

$$\int_{s_1}^{s_2} s \chi(s) ds = d \quad (6)$$

3. CONCLUDING REMARKS

The above formulae constitute a theoretical background to treat disordered solids with a special methodology based upon concepts related to signal theory. In this context, the cross-correlation function plays an important role; details about the physical meaning of this function can be found, for example, in Refs. [1–4]. In particular, expression (4) is very interesting. Finally, we can claim that randomness, which is a basic concept in the field of disordered solids, may be conceived in unusual ways in the light of the above exposition.

References

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