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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:

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

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:

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

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

From expression (2), it follows:

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

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:

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

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

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

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:

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

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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