TWO EXAMPLES OF ELECTRONIC SPECTRUM FLUCTUATIONS IN MICROPARTICLES

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We analyze the nearest-neighbour spacing distribution of the electronic spectrum of microparticles in two cases: a truncated octahedron consisting of 38 Ni atoms and a Ti catalytic complex formed by 24 atoms. In both cases a Poisson distribution is obtained.

The low-temperature thermodynamic and electromagnetic properties of electrons in small aggregates of atoms (such as microclusters or small metallic particles) depend on the spacing distribution of the electronic levels in the neighbourhood of the Fermi level [1]. It has been argued [2,3], without formal justification, that irregularities in the small particle surface will affect the level-spacing distribution. Kubo [2] assumed that a completely random sequence of levels would be obtained and, therefore, that the spectrum fluctuations would be of the Poisson type. On the other hand, Gor’kov and Eliashberg [3] assumed that surface irregularities, being of the order of atomic size, would induce random interactions of the electrons with the walls. These authors stated that this situation is analogous to that encountered in determining the distribution of high-excitation levels in nuclei, for which random-matrix theory is applicable [4]. If this last assumption is valid, the phenomena of level repulsion (i.e., the absence of small spacings in the distribution) will appear. It should be remarked that both approaches [2,3] were given the same qualitative justification, so a closer analysis is required to establish which

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Fig. 1. The distribution $P(x)$ of nearest-neighbour level spacings corresponding to the Ni-cluster d band [7]. The dependency of the 78 levels considered in the histogramme was not taken into account. The histogramme fits very well with the Poisson distribution $e^{-x}$, the probability of $x^2$ being 89%.

Nearest-neighbour spacing distribution, considering 58 levels around the Fermi level, is shown in Fig. 2, where it can be seen that it is again of the Poisson type. Both histogrammes were obtained after eliminating level density variations through an unfolding procedure [9].

From these two examples, in which the free-electron model was not assumed, we again obtain some indication that the Poisson spacing distribution might be more adequate to represent the electronic spectrum fluctuations in very small aggregates of atoms. It should be pointed out that a definite answer to this problem has certainly not been obtained from the theoretical point of view. A review [10] of the observed low-temperature properties of small particles also shows that the experimental situation is not at all clear. A definite answer will only come from the comparison of theoretical [11,12] and experimental results, which are now beginning to accumulate [1].

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References

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