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Existence of the Exponentially Localised Wannier Functions

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Abstract. A partial answer (Theorem 1 below) to a problem concerning analytic and periodic families of projections in Hilbert spaces is given. As a consequence the existence of exponentially localised Wannier functions corresponding to nondegenerated bands of arbitrary three-dimensional crystals is proved.

1. Statement of the Problem and the Result

The present note is motivated by one of the few basic questions of the quantum theory of periodic solids in the one-electron approximation which is not completely solved: the existence of exponentially localised Wannier functions [1, 2]. We shall consider only nondegenerated bands and neglect the spin (for the results obtained so far for degenerated bands, we refer to [3–5]). The Wannier functions falling off exponentially at infinity for arbitrary n-dimensional crystals. The proof is based on dimensional crystals [4, 6]; ii) n-dimensional crystals ($n > 1$) with a center of inversion [4]; iii) arbitrary crystals (i.e. with or without a centre of inversion) in the tight binding limit [4][1].

The result of this note is the existence of Wannier functions falling off exponentially at infinit for arbitrary n-dimensional crystals. The proof is based on a partial answer (Theorem 1 below) to the following problem concerning analytic families of projections in Hilbert spaces.

Problem P. *Let $\mathcal{H}$ be a separable Hilbert space, q be a positive integer,* $\mathcal{I}^q_a = \{\mathbf{z}^q = (z_1, \ldots, z_q) \in \mathbb{C}^q \,|\, |\mathrm{Im}\, z_i| < a,\ a > 0\}$ *and* $Q(\mathbf{z}^q): \mathcal{H} \to \mathcal{H}$ *be a projection-valued func-*

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1 There is a widespread opinion (see e.g. [2]) that the existence of exponentially localised Wannier functions has been proved for arbitrary n-dimensional crystals by Blount [7]. Unfortunately, this is not true since by his argument Blount proved *only* analyticity (as functions of the crystal momentum) of the Bloch functions, while for the exponential falling off the Wannier functions analyticity *and* periodicity of the Bloch functions is nedeed