Exponential decay properties of Wannier functions and related quantities

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In a classic paper, Kohn proved [1], for the case of a centrosymmetric crystal in one dimension (1D), that the Wannier functions (WFs) have an "exponential decay" $w(x) \sim e^{-hx}$, where the inverse decay length h is the distance of a branch point from the real axis in the complex k plane. More precisely, he showed that

$$\lim_{x\to\infty} w(x)\, e^{qx} = \begin{cases} 0, & q < h \\ \infty, & q > h \end{cases} .$$

However, this still allows an asymptotic decay of the form $w(x) \sim x^{-\alpha} e^{-hx}$ for *any exponent* α. Does such a power-law prefactor exist? We find [2] that indeed it does, and that the α value is universal for a given type of quantity in a given number of spatial dimensions. For example, in 1D, we present both analytical arguments and numerical evidence that the decay of the WFs is characterized by $\alpha = 3/4$, the decay of the density matrix obeys $\alpha = 1/2$, and the decay of non-orthogonal WFs (NWFs) constructed by a direct and dual construction technique are $\alpha = 1/2$ and $\alpha = 3/2$, respectively. We discuss efforts to construct NWFs with even better decay in the tails, but find that this leads to broader NWFs as measured by other criteria (e.g., second moments). Corresponding WFs and NWFs are also calculated numerically for Si in an empirical-pseudopotential framework in order to investigate the decay properties in 3D.

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[1] W. Kohn, Phys. Rev. **115**, 809 (1959).
[2] Lixin He and David Vanderbilt, Phys. Rev. Lett., in press.