

Abstract Submitted
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Exponentially localized quasi-free-particle generalized Wannier functions BRADLEY A. FOREMAN, Hong Kong University of Science and Technology — A new class of localized basis functions is proposed as a generalization of the Wannier functions for a free particle. The basis is orthonormal and its Fourier transform is given in explicit analytical form. For large values of the coordinate ($x \rightarrow \infty$), the wave functions are localized as $\exp(-Cx^\gamma)$, where $C > 0$ and $\frac{1}{2} \leq \gamma < 1$ are fixed constants (with the same value for each state in a given basis). In contrast, ordinary free-particle Wannier functions are localized only as $1/x$, while the Wannier functions for a crystal behave as $\exp(-C_n x)$, where C_n vanishes as the band index $n \rightarrow \infty$. Potential applications of the theory are discussed.

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