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Analytic structure of Bloch functions for linear molecular chains[1] EMIL PRODAN, PRISM, Princeton University — In this talk I will discuss Hamiltonians of the form $H = -\nabla^2 + v(x, y, z)$, with $v(x, y, z)$ periodic along the z direction, $v(x, y, z + b) = v(x, y, z)$. The wavefunctions of H are the well known Bloch functions $\psi_{n,\lambda}(x, y, z)$, with the fundamental property $\psi_{n,\lambda}(x, y, z + b) = \lambda\psi_{n,\lambda}(x, y, z)$ and $\partial_z\psi_{n,\lambda}(x, y, z + b) = \lambda\partial_z\psi_{n,\lambda}(x, y, z)$. I will give the generic analytic structure (i.e. the Riemann surface) of $\psi_{n,\lambda}(x, y, z)$ and their corresponding energy, $E_n(\lambda)$, as functions of λ. I will also discuss several applications, like a compact expression of the Green's function or the asymptotic behavior of the density matrix and other correlation functions for insulating molecular chains.

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[X] Prefer Oral Session
[ ] Prefer Poster Session

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