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The Kronig-Penney model extended to arbitrary potentials via numerical matrix mechanics

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We present a general method using matrix mechanics to calculate the bandstructure for 1D periodic potential arrays, filling in a pedagogical gap between the analytic solutions to the Kronig-Penney model and more complicated methods like tight-binding. By embedding the potential for a unit cell of the array in a region with periodic boundary conditions, we can expand in complex exponential basis states to solve for the matrix elements. We show that Bloch's condition can be added in a potential-independent way, and so repeated diagonalizations of the unit cell matrix with different parameters of the crystal momentum will fill out the bandstructure. Comparisons with the analytic solutions to the Kronig-Penney model show excellent agreement. We then generate bands for two variants of the Kronig-Penney model, the periodic harmonic oscillator and its inverted form, and a symmetric linear well such that each has similarly-bounded electrons at the peak of the third energy band. We show how these different, more "realistic", potentials can be used to tune electron-hole effective mass asymmetries. Finally, preliminary results for the extension to 2D are demonstrated.

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