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Periodic Numerical Grid Method for the Maximally Even Kronig-Penny Model JASON BYRD, RICHARD KRANTZ, Metropolitan State College of Denver — Energy band calculations for quasi-periodic crystals is an important field in condensed matter physics. Efficient and stable methods of calculation are necessary in the study of long quasi-periodic crystalline structures. The band gap structure of quasi-periodic crystals can be studied using a cell structure and applying a modified Kronig-Penney model. We show how a finite-element method using the discrete variable representation can be implemented with periodic boundary conditions on a Gauss-Lobatto Quadrature numerical grid. Because of the Gauss-Lobatto Quadrature numerical grid and the discrete variable representation, the local potential operators are represented as diagonal matrices and the kinetic energy matrix is quasi-block diagonal. This sparsity and block diagonal nature of the system greatly reduces the number of calculations necessary for the eigenvalue problem and increases the stability of the system as the size of the crystal chain grows. We implement the periodic finite-element discrete variable representation using a maximally even distribution of potentials as a modification to the usual Kronig-Penny model.

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