

Abstract Submitted  
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**Computational Physics in Undergraduate Solid State** JAVIER HASBUN, University of West Georgia — Computational physics is of essential importance in the undergraduate curriculum. In solid state physics the need to visualize complicated concepts and the need to understand difficult formulae demand the use of computers. Here, one of the most challenging tasks is to calculate the density of states of a solid, for example, where the band structure is needed. Integrations over the bands in k-space are quite challenging. I have developed an approach to this task and demonstrate the steps to carry out its computation suitable for undergraduate student use. The approach is applied to the simple cubic structures. The method used is based on employing the band structure's Green's function and employing the k-space Brillouin-zone ray approach [1] combined with a complex integration method [2]. Because the Green's function contains information about the system's spectrum, the density of states can naturally be used for this purpose. The number of occupied electron states up to a certain energy is obtained using Romberg's method and the results are shown for the above example structures. Other solid state properties that can be illustrated will be discussed.

[1] An-Ban Chen, Phys. Rev. B, Vol. 16, 3291 (1977). [2] Hasbun, Javier, <http://meetings.aps.org/link/BAPS.2009.MAR.L29.12>

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