

Abstract Submitted
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Accurate quantum states for a 2D-dipole DANIEL VRINCEANU,
Texas Southern University — Edge dislocations are crucial in understanding both mechanical and electrical transport in solid and are modeled as linear distributions of dipole moments. The calculation of the electronic spectrum for the two dimensional dipole, represented by the potential energy $V(r, \theta) = p \cos(\theta)/r$ has been the topic of several studies that show significant difficulties in obtaining accurate results. In this work we show that the source of these difficulties is a logarithmic contribution to the behavior of the wave function at the origin, that was neglected by previous authors. By taking into account this non-analytic deviation of the solution of Schrödinger's equation superior results, with the expected rate of convergence, are obtained. This goal is accomplished by “adapting” general algorithms for solving partial derivative differential equations to include the desired asymptotic behavior. We demonstrate this principle for the variational principle and finite difference methods.

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