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(U*) Calculation of High Harmonic Spectrum from a 1D periodic potential

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In this research project, I calculated the high-harmonic spectrum from a 1D periodic potential. I investigated numerical methods for solving the 1D time-dependent Schrodinger equation of a particle in a double-well potential, as well as determining its ground state. I used the Crank Nicolson method [1], which is a finite difference method that can be used for numerically solving second-order partial differential equations. Using this method, I calculated the time evolution of an electronic wave function in a harmonic potential. My code was bench-marked against analytic solutions of the harmonic oscillator wave functions. I extended the use of this code by implementing the imaginary time method [2] to determine the ground state of an electron in a double-well potential. The time-independent Schrodinger equation is solved in the Bloch state basis to calculate the band structure of two different 1D periodic potentials. The calculations of dispersion relation are used to calculate the High Harmonic Spectrum and the final results are compared with [3].

[1] Wachter, C. (2017). Numerical Solution of the Time-Dependent 1D-Schrodinger Equation using Absorbing Boundary Conditions (Bachelor Thesis, University of Graz, Austria). Retrieved from https://physik.uni-graz.at/˜pep/Theses/BachelorThesis_Wachter_2017.pdf

[2] Williamson, A. (1996). Quantum Monte Carlo Calculations of Electronic Excitations.
Retrieved from http://www.tcm.phy.cam.ac.uk/˜ajw29/thesis/node27.html

[3] Wu, M. (2015). Attosecond Transient Absorption in Gases and High Harmonic Generation in Solids (Doctoral dissertation, Louisana State University, USA). Retrieved from https://digitalcommons.lsu.edu/cgi/viewcontent.cgi?article=4320&cont

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