First Principle 2017-Fall midterm Solution

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1. Al band structure using GGA calculation and free-electron band structure.
2. Kohn-Sham
3. Car-Parrinelo EOM
4. GGA, GGA+U of MnO in AF-II
5. Finite difference algorithms.

   In the following, we evaluate the harmonic oscillator with "Euler" , "Predictor-Corrector" and "Velocity-verlet" method.

   (a) Euler method with $dt = 2.5e - 3\pi$, $x(0) = 1$,$v(0) = 0$

   (b) Euler method with $dt = 2.5e - 4\pi$, $x(0) = 1$,$v(0) = 0$
   compare the result with (a), we can see that reducing the update time interval, the energy still not conserved, but the error is decreased.

   (c) Euler method compare with Predictor-Corrector method with $dt = 2.5e-3\pi$, $x(0) = 1$,$v(0) = 0$
   compare the result with (a), we can see that with the same update time interval (dt), we can see that the energy increment error is significantly reduced.

   (d) Euler method compare with Velocity-Verlet method with $dt = 2.5e - 3\pi$, $x(0) = 1$,$v(0) = 0$
   compare the result with (a), we can see that with the same update time interval (dt), we can see that the energy increment error is reduced.

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