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COMPUTER LABORATORY SESSION

OPTIMIZED POTENTIALS FOR PERIODIC SYSTEMS - FITPN

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These are preliminary lecture notes, intended only for distribution to participants.

OPTIMIZED POTENTIALS FOR PERIODIC SYSTEMS - FITPN

For extended systems, periodic boundary conditions are the common choice for extrapolating results of a finite system to the thermodynamic limit. Whereas for short-range potentials, the minimum image convention is in general sufficient, long-range potentials have to be treated differently. For the potential $v(r)$ for an infinite system in D spatial dimensions,

$$v(r) = \int \frac{d^D k}{(2\pi)^D} e^{ikr} \tilde{v}(k), \tag{1}$$

the "best" potential of the finite system of length L is given by

$$v_L(r) = \frac{1}{L^D} \sum_k e^{ikr} \tilde{v}(k) = \sum_n v(r + nL). \tag{2}$$

Since long-range potentials converge slowly in k and in real space, the key idea is to split the potential into a k-space part and a real space part

$$v_L(r) = \sum_n v_{sr}(r + nL) + \frac{1}{L^D} \sum_k e^{ikr} \tilde{v}_{lr}(k) \tag{3}$$

and determine the short range part $v_{sr}(r)$ and the long-range part $\tilde{v}_{lr}(k)$ such that both summations are rapidly convergent, and the minimum image convention is sufficient to approximate the first sum over images containing $v_{sr}(r)$.

FITPN provides this division of any function into optimized short-range and long-range potentials, using the procedure proposed by Natoli and Ceperley [1].

The INPUT is the Fourier transform of the desired function on a grid of k-points $\tilde{v}(k)$ together with some options such as the cutoff radius in r-space and the possibility of imposing "cusp"-conditions at the origin,
The OUTPUT are a spline for the short range function and the table of the long-range potential $\tilde{v}_{lr}(k)$ for $k \leq K_c$.

RUNNING *fitpn* provides a small DEMONSTRATION allowing you to compute the optimized potentials for the Coulomb $1/r$ potential and the RPA-Jastrow potential in 3 dimensions. As INPUT you have to give the number of intervals for the spline-function $(1, \ldots, 30)$, and the number of k-shells $(0, \ldots, 25)$ which determines the cut-off K_c in k-space. As OUTPUT, the files *optimized_pot.vr* and *optimized_pot.vk* provide the optimized potentials in r and k space in the format $(r,\ v_{sr}(r),\ r * v_{sr}(r))$ and $(k,\ v_{lr}(k))$.

The "classic" way to treat the Coulomb-potential in three dimensions is the EWALD summation method. The split up is done using Gaussian charge distributions allowing you to analytically determine v_{sr} and $\tilde{v}_{lr}(k)$,

$$v_{sr}(r) = \frac{erfc(\kappa r)}{r} \tag{4}$$

$$\tilde{v}_{lr}(k) = \frac{4\pi}{k^2} e^{-(k/2\kappa)^2} \tag{5}$$

where κ is a convergence parameter to be determined such that the image sum in real space and the k-space summation is converging rapidly. (Note that the Coulomb potential is a special case where an analytical result is known.)

- Run *fitpn*.
  - Fix the number of k-shells (corresponds to K_c). How does the number of k-vectors with $|k| \leq K_c$ increase with the number of k-shells?
  - Vary the number of intervals used for the splines of the short range function. The χ^2 value resulting for the fit of the true periodic potential are written out. How do you have to chose the number of spline intervals for a given K_c?

- For the Coulomb-potential the result of the optimized potential may be judged by comparing the computed Madelung constant with the value for a cubic lattice found in the literature. The Madelung constant is given by the potential of a single charge interacting with all of his image charges (without the self-energy), $v_{mad} = \lim_{r \to 0}(v_L(r) - 1/r)$. How to calculate v_{mad} using the analytical Ewald-potential?
- RUNNING *ewald* calculates the Ewald-Coulomb-potential. The convergence parameter κ has to be given and also the number of k-shells used in Fourier space. Short and long range potentials are written to the files *ewald_pot.vr* and *ewald_pot.vk*. In the standard output are also given the value of the short-range function at $L/2$ and the value of the long-range function at $k = K_c$.
  - Chose κ such that the minimum image convention can be used. Compare the resulting potentials with the optimized potentials of FITPN.

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[1] V. Natoli and D.M. Ceperley, Comput. Physics 117, 171 (1995).