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Determining nearest image in non-orthogonal periodic systems.

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The simulation of crystalline systems where the crystal axes are non-orthogonal, raises the question of finding the nearest image of a particle. Smith has recently showed [1] that if a suitably chosen spherical cutoff is imposed on the interactions then the nearest image can be conveniently determined in the non-orthogonal system defined by the crystal axes and then simply transformed back to the orthogonal laboratory frame. The purpose of this note is to describe a relatively simple procedure to find the nearest image without the imposition of the spherical cutoff.

Assume that the columns of the matrix **H** contain the vectors spanning (in the orthogonal system) the unit cell corresponding to the nonorthogonal system. The coordinates of a point in the orthogonal system, $\underline{x}$, are given as

$$\underline{x} = \mathbf{H}\underline{s} \tag{1}$$

where $\underline{s}$ gives the fractional coordinates of the same point in the non-orthogonal system ($|s_\mathrm{k}| \leq 1$ for points inside the cell). Assume that a particle is in the center of the cell that is also the center of the coordinate system. A point $\underline{s}$ is to be examined if it possesses an image that might be nearer to the center. The various images of $\underline{s}$ can be described as

$$\mathbf{H}\underline{s} + \sum_{\mathrm{k}=1}^{\mathrm{d}} c_\mathrm{k}\underline{H}_\mathrm{k} \tag{2}$$

where d is the dimension of the space (e.g., three for crystals) and c_k is either -1, 0 or 1. Thus the distance of an image described by $\underline{c}$ is

$$|\mathbf{H}\underline{s} + \sum_{\mathrm{k}=1}^{\mathrm{d}} c_\mathrm{k}\underline{H}_\mathrm{k}|^2 =$$

$$|\mathbf{H}\underline{s}|^2 + \sum_{\mathrm{k,l}=1}^{\mathrm{d}} c_\mathrm{k}c_\mathrm{l}(\underline{H}_\mathrm{k} \cdot \underline{H}_\mathrm{l}) + 2\sum_{\mathrm{k}=1}^{\mathrm{d}} c_\mathrm{k}(\underline{H}_\mathrm{k} \cdot \mathbf{H}\underline{s}) = \tag{3}$$

$$|\underline{x}|^2 + \sum_{\mathrm{k,l=1}}^{\mathrm{d}} c_{\mathrm{k}} c_{\mathrm{l}} (\underline{H}_{\mathrm{k}} \cdot \underline{H}_{\mathrm{l}}) + 2 \sum_{\mathrm{k=1}}^{\mathrm{d}} c_{\mathrm{k}} (\underline{s} \cdot \underline{H}^2_{\mathrm{k}}) \tag{4}$$

Here $\underline{H}^2_{\mathrm{k}}$ stands for the k-th column of the square of the matrix $\mathbf{H}$. As described in [1], simple translations along the non-orthogonal axes can ensure that the point $\underline{s}$ will be inside the unit cell and if its distance from the center (the first term in (3) and (4)) is less than the smallest half-width of the unit cell then it will be the nearest image. For larger distances, however, images outside the simulation cell may lie closer to the cell center. In this case, more work is needed to obtain the values of $\underline{c}$ that minimize (4).

The first term is independent of $\underline{c}$ and therefore will not affect the minimum. The second term depends only on $\underline{c}$ and the cell axes and therefore it can be calculated once at the beginning of the calculations for all 3^{d} possible $\underline{c}$. The last term contains d different coefficients that depend on $\underline{s}$ — these have to be calculated each time. The number of possibilites to be examined can be further reduced from 3^{d} to 2^{d} by recognizing that for each direction k, c_{k} can be only 0 or -SIGN(s_{k}) since $\underline{s}$ is already assumed to be translated inside the cell. We are thus left with comparing 2^{d} values of the type

$$S(\underline{c}) + (\underline{c} \cdot \underline{B}) \tag{5}$$

where B_{k}=$2(\underline{s} \cdot \underline{H}^2_{\mathrm{k}})$. As half of the c_{k}'s to be considered is zero, (5) can be evaluated rather fast for the 2^{d} cases.

Once the value of c_{k} minimizing (4) is obtained, the nearest image can be simply obtained as

$$\mathbf{H}\underline{s} + \underline{c} H_{\mathrm{k}}. \tag{6}$$

The second term can again be prepared at the beginning of the calculation for all 3^{d} possible $\underline{c}$.

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Reference:

1. W. Smith, Information Quartely for Computer Simulation of Condensed Matter, No 30, Apr. (1989).