# 3D Image Reconstruction Hamiltonian Method for Phase Recovery ${ }^{1}$ 

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Submitted to Phys. Rev. B

Abstract:

The problem of reconstructing a positive semi-definite 3-D image from the measurement of the magnitude of its 2-D fourier transform at a series of orientations is explored. The phase of the fourier transform is not measured. The algorithm developed here utilizes a Hamiltonian, or cost function, that at its minimum provides the solution to the stated problem. The energy function includes both data and physical constraints on the charge distribution or image.

PACS numbers: 61.10.Eq, 42.30.Rx, 42.30.Wb, 81.07.Bc

[^0]
## 1 Introduction and Motivation

The problem of recontructing an image from the measured magnitude of its fourier transform in the Fraunhofer diffraction regime is discussed here. This, in turn, involves reconstructing the unknown phases based on general properties of the image such as positivity and finite extent [1]. The terms image, object, and charge distribution will be used interchangeably in this note.

The determination of structure from a set of patterns measured from a 3-D object at known orientations has been well discussed and has been treated by a number of authors, see references $[2,3,4,5,6]$, where other citations can be found.

The possibility of determining the structure of a single molecule by measurements using a coherent x-ray source[7] has been proposed by Miao, Hodgson and Sayre [8] and Miao, Ishikawa, Anderson and Hodgson [9]. In these papers the oversampling ratio $\sigma$ was introduced, the importance of measurements at many different orientations, and uniqueness of the resulting solution are discussed. These papers were the inspiration for the present work.

In a previous note, a method for determining the orientations of each pattern was described that used the familiar concept of 'common' or 'matching' lines in the measured Fourier magnitudes[10]. In this note, a new method is presented for constructing the image once the orientations are determined. The present algorithm utilizes a Hamiltonian or energy function that yields the desired solution when minimized. The Hamiltonian can be augmented by extra constraints that impose additional physical requirements on the extracted image.

One example of such an additional constraint is to extract the most compact image that fits the given data. As has been discussed [9], in particular footnote 20, if the long wave length or small $\vec{k}_{\perp}$ sector of the pattern is not available, the resulting loss of information on the long distance features of the image allows the image to expand, or at least to be uncertain, near its outer boundary. The imposition of this minimal size constraint allows one to explore the error introduced by such missing data.

The 3-D diffraction pattern from a coherent x-ray beam is given in the Fraunhofer scattering region as

$$
\begin{equation*}
F[\mathbf{k}]=M[\mathbf{k}] \exp (-i \phi[\mathbf{k}])=\sum_{\vec{r}} \exp [-i \mathbf{k} \cdot \tilde{\mathbf{r}}] v[\tilde{r}] \tag{1}
\end{equation*}
$$

where $M[\mathbf{k}]$ is the magnitude of the pattern, $\phi[\mathbf{k}]$ its phase, and $v[\vec{r}]$ is the charge distribution, which will also be termed the image or the object. If both $M[\mathbf{k}]$ and $\phi[\mathbf{k}]$ were measurable, then $v[\vec{r}]$ can be computed directly from the inverse transform. However the full 3-D transform cannot be directly measured. It must be constructed from a series of 2-D patterns measured from the target at many different orientations. A final problem is that the phase of the 2-D patterns cannot be measured and are unknown. They must be inferred from the data and known physical properties of the image.

For simplicity, several notational abbreviations will be introduced. Following the formulation used in reference [9], the Fourier components of the object will be sampled at a finer spacing than the Nyquest frequency. The three k components will each range from $-I<=k<=I$ with the total number of points given by $N=2 * I+1$ with volume $V=N^{3}$. A smaller volume $V_{o}$ will be introduced, which nevertheless is chosen to be large enough to completely contain the object. Each coordinate of the object will be restricted to a smaller range, $-I_{o}<=i<=I_{o}$, where $I>I_{o}$ and $N_{o}=2 * I_{o}+1$ with volume $V_{o}=N_{o}^{3}$. The object is defined to be real for the problem considered here, and to be zero identically outside the volume $V_{o}$. The oversampling ratio is defined as

$$
\begin{equation*}
\sigma=V / V_{o} \tag{2}
\end{equation*}
$$

Note that as this ratio increases, the more information is being supplied about the object, namely that the charge distribution is zero in the growing region $\left(V-V_{o}\right)$. This added information on the object can make up for a lack of experimental information on the phase of the Fourier transform. In several studies of 3-D image reconstruction [9, 11], it was found that $\sigma>2$ was necessary for reconstruction, and $\sigma \approx 3$ produced reasonable output images.

Thus the coordinate point becomes $\vec{r}=(i, j, k)$ and a volume integral is written as

$$
\begin{equation*}
\int d^{3} r v[\vec{r}]=\sum_{i=-I_{o}}^{i=I_{o}} \sum_{j=-I_{o}}^{j=I_{o}} \sum_{k=-I_{o}}^{k=I_{o}} v[i, j, k] \equiv \sum_{\vec{r}<V_{o}} v[\vec{r}] . \tag{3}
\end{equation*}
$$

## 2 Data Description

The data is presented for analysis in a tomographic form. 2-D Patterns are measured at a set of different orientations of a 3-D object or image. These patterns are projected Fourier transforms of the image. For completeness, a review of our definition of the discrete Fourier transform is given in Appendix A. The Fourier pattern from a source in the 'standard' orientation will be written as

$$
\begin{align*}
F\left[\vec{k}_{\perp}\right] & =\sum_{\vec{r}} \exp \left[-i \vec{k}_{\perp} \cdot \vec{r}\right] v[r] \\
& =\sum_{r_{\perp}} \exp \left[-i \vec{k}_{\perp} \cdot r_{\perp}\right] \sum_{z} v[\vec{r}] \tag{4}
\end{align*}
$$

where the second form emphasizes that the 2-D pattern is a longitudinal projection of the object. The Fourier pattern from a source rotated by the matrix $R$ is

$$
\begin{align*}
F_{R}\left[\vec{k}_{\perp}\right] & =\sum_{\vec{r}} \exp \left[-i \vec{k}_{\perp} \cdot \vec{r}\right] v\left[\vec{R}^{T} r\right] \\
F_{R}\left[\vec{k}_{\perp}\right] & =\sum_{\vec{r}} \exp \left[-i \vec{k}_{\perp} \cdot \vec{R} \cdot \vec{r}\right] v[\vec{r}] . \tag{5}
\end{align*}
$$

Write $\vec{k}_{\perp}=\left(k_{x}, k_{y}, 0\right)$ so that

$$
\begin{align*}
\vec{k}_{\perp} \cdot \vec{R} \cdot \vec{r}= & k_{x}[R(x, x) x+R(x, y) y+R(x, z) z] \\
& +k_{y}[R(y, x) x+R(y, y) y+R(y, z) z] \tag{6}
\end{align*}
$$

The data is given by the series of patterns $1 \leq n \leq N$ with

$$
\begin{equation*}
F_{n}\left[\vec{k}_{\perp}\right]=M_{n}\left[\vec{k}_{\perp}\right] \exp \left[-i \phi_{n}\left[\vec{k}_{\perp}\right]\right]=\sum_{\vec{r}} \exp \left[-i k_{\perp} \cdot \vec{R}_{n} \cdot r\right] v[\vec{r}], \tag{7}
\end{equation*}
$$

where the phases $\phi_{n}\left[\vec{k}_{\perp}\right]$ are not measured. In another note, a technique for determining the rotation matrices $\vec{R}_{n}$ was described. This method involves examination and analysis of the matching lines, otherwise termed the common lines, of the measured Fourier magnitudes $M_{n}\left[\overrightarrow{k_{\perp}}\right]$. It is assumed that this has been done and that all rotation matrices $\vec{R}_{n}$ are known. Note that $F_{n}[0]=F_{m}[0]$ for all pairs $n$ and $m$, since each is the volume integral of the object, and that a measure of the average value of the image inside $V_{o}$ is given directly by the data

$$
\begin{equation*}
\langle v[\vec{r}]\rangle=\frac{1}{N V_{o}} \sum_{n} F_{n}(0) . \tag{8}
\end{equation*}
$$

The Problem: For a given magnitude $M_{n}\left[\overrightarrow{k_{\perp}}\right]$ and the fact that the image has compact support, find the set of phases $\phi_{n}\left[\vec{k}_{\perp}\right]$, or rather $\cos \phi_{n}\left[\vec{k}_{\perp}\right]$ and $\sin \phi_{n}\left[\vec{k}_{\perp}\right]$, that yield a positive semidefinite real image $v[\vec{r}]$ and determine that image.

This statement of the problem is in the language of the phase iteration method used by Fienup [1], Miao et al. [8] and others. It is the purpose of this note to provide an alternative formulation of the problem and to describe a simple, certainly not the most efficient nor the only, solution method. Our algorithm utilizes an energy function $H$ that must be minimized in the presence of inequality constraints.

## 3 Hamiltonian Formulation

In order to simplify the equations, the following definitions are introduced, recall Eq. [7], as sums on the lattice:

$$
\begin{align*}
& C_{n}\left[\vec{k}_{\perp}\right]=\sum_{\vec{r}} v[\vec{r}] \cos \left[\vec{k}_{\perp} \cdot \vec{R}_{n} \cdot \vec{r}\right]  \tag{9}\\
& S_{n}\left[\vec{k}_{\perp}\right]=\sum_{\vec{r}} v[\vec{r}] \sin \left[\vec{k}_{\perp} \cdot \vec{R}_{n} \cdot \vec{r}\right] \tag{10}
\end{align*}
$$

and the measured magnitude of the pattern to be fit by an appropriate choice of $v[\vec{r}]$ is given by

$$
M_{n}\left[\overrightarrow{k_{\perp}}\right]^{2}=C_{n}\left[\vec{k}_{\perp}\right]^{2}+S_{n}\left[\vec{k}_{\perp}\right]^{2}
$$

If there were no constraints on the image, one suitable energy functional that at its minimum would determine $v[r]$ would be

$$
\begin{equation*}
h(v[\vec{r}])=\frac{1}{4} \sum_{n} \sum_{\vec{k}_{\perp}}\left\{C_{n}\left[\vec{k}_{\perp}\right]^{2}+S_{n}\left[\vec{k}_{\perp}\right]^{2}-M_{n}\left[\overrightarrow{k_{\perp}}\right]^{2}\right\}^{2} . \tag{11}
\end{equation*}
$$

However, this form seems to be quite sensitive during the minimization process although there may be procedures that can eliminate this difficulty.

A superior form of the energy functional is

$$
\begin{equation*}
H(v[\vec{r}])=\frac{1}{2} \sum_{n} \sum_{\vec{k}_{\perp}}\left\{\sqrt{C_{n}\left[\vec{k}_{\perp}\right]^{2}+S_{n}\left[\vec{k}_{\perp}\right]^{2}}-M_{n}\left[\overrightarrow{k_{\perp}}\right]\right\}^{2} \tag{12}
\end{equation*}
$$

The positivity constraint will be imposed later, but first $H$ will again be minimized by determining the optimum global normalization of any given image distribution $v[\vec{r}]$. Set $v[\vec{r}] \rightarrow w v[\vec{r}]$ so that

$$
\begin{equation*}
H(v[\vec{r}]) \rightarrow \frac{1}{2} \sum_{n} \sum_{\vec{k}_{\perp}}\left\{w \sqrt{C_{n}\left[\vec{k}_{\perp}\right]^{2}+S_{n}\left[\vec{k}_{\perp}\right]^{2}}-M_{n}\left[\overrightarrow{k_{\perp}}\right]\right\}^{2} \tag{13}
\end{equation*}
$$

The minimum with respect to $w$ yields

$$
\begin{equation*}
w \sum_{n} \sum_{\vec{k}_{\perp}}\left\{C_{n}\left[\vec{k}_{\perp}\right]^{2}+S_{n}\left[\vec{k}_{\perp}\right]^{2}\right\}=\sum_{n} \sum_{\vec{k}_{\perp}} M_{n}\left[\overrightarrow{k_{\perp}}\right] \sqrt{C_{n}\left[\vec{k}_{\perp}\right]^{2}+S_{n}\left[\vec{k}_{\perp}\right]^{2}} \tag{14}
\end{equation*}
$$

In the following, $v[\vec{r}], C_{n}\left[\vec{k}_{\perp}\right]$ and $S_{n}\left[\vec{k}_{\perp}\right]$ are to be renormalized by the factor $w$ which is absorbed into their definition.

The normalization factor $w$ can be simplified, or rather approximated, by restricting the $\vec{k}_{\perp}$ sum over a suitably chosen region in which $M_{n}\left[\overrightarrow{k_{\perp}}\right]$ is large. For example, if only the volume integral of the trial image is required to agree with the average measured value, then only the single point $\vec{k}_{\perp}=0$ needs to be included in the sum. Then the approximate $w$ becomes

$$
\begin{equation*}
w \sum_{n}\left\{C_{n}[0]^{2}+S_{n}[0]^{2}\right\} \approx \sum_{n} M_{n}[0] \sqrt{C_{n}[0]^{2}+S_{n}[0]^{2}} \tag{15}
\end{equation*}
$$

Recall that the constraints on an allowable image are that

$$
\begin{equation*}
v[\vec{r}]=0 \quad \text { for } \vec{r}>\vec{V}_{o} \quad \text { and } \quad v[\vec{r}] \geq 0 \quad \text { for } \vec{r}<\vec{V}_{o}, \tag{16}
\end{equation*}
$$

where $\vec{V}_{o}$ is a region that is large enough to definitely contain the object. Thus the integral over $\vec{r}$ in Eqs. [21] and [22] is only over the interior of $\vec{V}_{o}$. The positivity constraint will be enforced by adding a term to the Hamiltonian of the form

$$
\begin{equation*}
\delta H=-\sum_{\vec{r}} \lambda(\vec{r}) v[\vec{r}], \tag{17}
\end{equation*}
$$

where $\lambda(\vec{r})$ is a positive inequality multiplier. $\lambda\left(\vec{r}<\vec{V}_{o}\right)$ is a non-negative inequality multiplier that is zero if $v[\vec{r}]$ is positive, and is chosen to make $v[\vec{r}] \geq 0$ inside the allowed region [12]. Inequality multipliers are discussed in, for example, reference[13]. Note that this term is identically zero at the minimum, and therefore does not change the value of $H$ at this point.

Energy: The energy function is a function of the pattern data, the orientation of each pattern and the unknown image values as well as the constraint parameters. Consider the form

$$
\begin{equation*}
H(v[\vec{r}])=\frac{1}{2} \sum_{n} \sum_{\vec{k}_{\perp}}\left\{\sqrt{C_{n}\left[\vec{k}_{\perp}\right]^{2}+S_{n}\left[\vec{k}_{\perp}\right]^{2}}-M_{n}\left[\overrightarrow{k_{\perp}}\right]\right\}^{2}-\sum_{\vec{r}} \lambda(\vec{r}) v[\vec{r}] \tag{18}
\end{equation*}
$$

where the factor of $w$ has been absorbed into $v[\vec{r}], C_{n}\left[\vec{k}_{\perp}\right]$ and $S_{n}\left[\vec{k}_{\perp}\right]$.
Consider the variation of the energy with respect to the image value at a point

$$
\begin{equation*}
\frac{\delta H}{\delta v[\vec{r}]}=\sum_{n} \sum_{\vec{k}_{\perp}} j_{n}\left(\vec{k}_{\perp}, \vec{r}\right)-\lambda(\vec{r}), \tag{19}
\end{equation*}
$$

where the auxiliary quantity $j_{n}$ has been introduced as

$$
\begin{align*}
j_{n}\left(\vec{k}_{\perp}, \vec{r}\right)= & \frac{\sqrt{C_{n}\left[\vec{k}_{\perp}\right]^{2}+S_{n}\left[\vec{k}_{\perp}\right]^{2}}-M_{n}\left[\overrightarrow{k_{\perp}}\right]}{\sqrt{C_{n}\left[\vec{k}_{\perp}\right]^{2}+S_{n}\left[\vec{k}_{\perp}\right]^{2}}} \times \\
& \left\{C_{n}\left[\vec{k}_{\perp}\right] \cos \left[k_{\perp} \cdot \vec{R}_{n} \cdot r\right]+S_{n}\left[\vec{k}_{\perp}\right] \sin \left[k_{\perp} \cdot \vec{R}_{n} \cdot r\right]\right\} \tag{20}
\end{align*}
$$

If $C_{n}\left[\vec{k}_{\perp}\right]=S_{n}\left[\vec{k}_{\perp}\right]=0$ at an isolated value of $\vec{k}_{\perp}$, then a direct evaluation leads to $j_{n}\left(\vec{k}_{\perp}, \vec{r}\right)=$ $-M_{n}\left[\overrightarrow{k_{\perp}}\right]$.

## 4 Additional Constraints

An example of an additional constraint that can be imposed using the Hamiltonian approach but which seems difficult to implement with the phase iteration method will be discussed briefly. This particular constraint is used to explore the effect described in Section I of missing data, especially
the forward direction, small $\vec{k}_{\perp}$ data. In order to determine the most compact but positive image that satisfies the data, consider adding to the Hamiltonian the two constraints

$$
\begin{equation*}
\delta H=+\sum_{\vec{r}} v[\vec{r}]\left\{-\lambda(\vec{r})+\nu \vec{r}^{2}\right\}, \tag{21}
\end{equation*}
$$

where $\lambda(\vec{r})$ is the familiar positive inequality multiplier and $\nu$ is a positive parameter that encourages $v[\vec{r}]$ to be as compact as possible. The factor $\vec{r}^{2}=i_{x}^{2}+i_{y}^{2}+i_{z}^{2}$ could also be replaced by the less drastic term $|\vec{r}|=\left|i_{x}\right|+\left|i_{y}\right|+\left|i_{z}\right|$.

The variation of the energy with respect to the image value at a point then takes the form

$$
\begin{equation*}
\frac{\delta H}{\delta v[\vec{r}]}=\sum_{n} \sum_{\vec{k}_{\perp}} j_{n}\left(\vec{k}_{\perp}, \vec{r}\right)-\lambda(\vec{r})+\nu \vec{r}^{2} \tag{22}
\end{equation*}
$$

One might start the iteration with $\nu=0$ and then as the image is iteratively determined, increase $\nu$ to explore changes in the image induced by the additional constraint.

Another physical constraints that could be added are similar to a maximum entropy constraint, namely to find the smoothest image that fits the given data. One way to accomplish this is to add a term involving the sum over the object of the square of the gradient of the image. Another approach is to add an entropy type term.

## 5 Minimization Scheme

Assume that there is a tentative (guess) image $v_{0}[\vec{r}]$. Improvements to this image are computed by expanding $v[\vec{r}]$ (recall that $\vec{r}<\vec{V}$ ):

$$
\begin{equation*}
H(v[\vec{r}])=H\left(v_{0}[\vec{r}]+\delta v[\vec{r}]\right)=H\left(v_{0}[\vec{r}]\right)+\delta v[\vec{r}] \frac{\partial H(v[\vec{r}])}{\partial v[\vec{r}]} . \tag{23}
\end{equation*}
$$

In this steepest descent iteration, if the derivative of the Hamiltonian is negative (positive) then one increases (decreases) the image at the point $\vec{r}$. If the tentative image is negative then it is always increased to zero by the appropriate choice of the positive definite parameter $\lambda(\vec{r})$.

Schema: Guess an image $v_{0}[\vec{r}]$ that satisfies the requisite conditions. Initialize the restraint parameter $\lambda(\vec{r})$ to zero and choose an iteration step parameter $\eta>0$. Compute the 2-D quantities $C_{n}\left[\vec{k}_{\perp}\right]$ and $S_{n}\left[\vec{k}_{\perp}\right]$ for $(1 \leq n \leq N)$ using $v_{0}[\vec{r}]$ and the known $\vec{R}_{n}$. Then

1. Evaluate the scale factor $w$ and renormalize $v[\vec{r}], C_{n}\left[\vec{k}_{\perp}\right]$ and $S_{n}\left[\vec{k}_{\perp}\right]$.
2. Choose a lattice point $\vec{r}_{i}=\left(i_{x}, i_{y}, i_{z}\right)$.
3. Compute $H^{\prime}\left(\vec{r}_{i}\right)$, the derivative of $H$ w.r.t. $v\left[\vec{r}_{i}\right]$, using Eq. [19].
4. If $H^{\prime}\left(\vec{r}_{i}\right)$ is not 0 , tentatively replace

$$
\begin{equation*}
v\left[\vec{r}_{i}\right] \rightarrow v\left[\vec{r}_{i}\right]+\delta v\left[\vec{r}_{i}\right] \quad \text { where } \quad \delta v\left[\vec{r}_{i}\right]=-\eta H^{\prime}\left(\vec{r}_{i}\right) . \tag{24}
\end{equation*}
$$

If the new $v\left[\vec{r}_{i}\right] \geq 0$ with $\lambda\left(\vec{r}_{i}\right)=0$, set $\lambda\left(\vec{r}_{i}\right)=0$. If not, choose $\lambda\left(\vec{r}_{i}\right)$ so that the new $v\left[\vec{r}_{i}\right]=0$.
5. If $v\left[\vec{r}_{i}\right]$ has changed at $\vec{r}_{i}$, update $C_{n}\left[\vec{k}_{\perp}\right]$ and $S_{n}\left[\vec{k}_{\perp}\right]$ at all $\vec{k}_{\perp}$ via

$$
\begin{align*}
C_{n}\left[\vec{k}_{\perp}\right] & \rightarrow C_{n}\left[\vec{k}_{\perp}\right]+\delta v\left[\vec{r}_{i}\right] \cos \left[\vec{k}_{\perp} \cdot \vec{R}_{n} \cdot \mathrm{r}_{\mathrm{i}}\right]  \tag{25}\\
S_{n}\left[\vec{k}_{\perp}\right] & \rightarrow S_{n}\left[\vec{k}_{\perp}\right]+\delta v\left[\vec{r}_{i}\right] \sin \left[\vec{k}_{\perp} \cdot \vec{R}_{n} \cdot \mathrm{r}_{\mathrm{i}}\right] . \tag{26}
\end{align*}
$$

6. Return to Step 2 and repeat for a new lattice point.
7. After all lattice points have been examined, return to step 1 .

Alternative orderings of these iteration steps can be used. For example, the order of step 5 and 6 can be inverted.

Once the minimum of $H$ has been found, the image is given by $v[\vec{r}]$, while the phase of the transform is given in terms of $C_{n}\left[\vec{k}_{\perp}\right]$ and $S_{n}\left[\vec{k}_{\perp}\right]$.

Orientation Check: The scheme described here requires that the orientation of each pattern be known and this task was described separately. In order to check this determination, which is subject to errors arising from pattern intensity and noise, one may add to the above steps an examination of each individual pattern error

$$
\begin{equation*}
\operatorname{err}(n)=\sum_{\vec{k}_{\perp}}\left\{\sqrt{C_{n}\left[\vec{k}_{\perp}\right]^{2}+S_{n}\left[\vec{k}_{\perp}\right]^{2}}-M_{n}\left[\vec{k}_{\perp}\right]\right\}^{2} \tag{27}
\end{equation*}
$$

If this quantity is found to be large for a particular pattern $n$, after the iteration has had a chance to partially converge, one may assume that it could be due to an poor determination of the pattern orientation. Therefore go into the $R_{n}(\psi, \theta, \phi)$, redetermine the euler angles to minimize $\operatorname{err}(n)$ for the approximate image as given at that stage of the iteration, and then resume the full iteration scheme.

Local Minima: To help the above scheme avoid and to test for local minima, it is possible to insert a roughening step into the iteration scheme. After a given number of iterations steps, a random variation can be added to the image at every point $\vec{r}$. That is, $v[\vec{r}] \rightarrow v[\vec{r}]+\sigma\langle v[\vec{r}]\rangle$, where $\langle v[\vec{r}]\rangle$ given by Eq. [8]. $\sigma$ is a random variable satisfying $-f<\sigma<f$ and the scale fraction satisfies $0<f<1$. The fraction $f$ should start out less than one and be allowed to decrease as the iteration converges.

## 6 Results and Conclusions

The above formulation was implemented in a program written in C++ and a few small test cases were run. A typical case used a full lattice of size $N=15$, i.e., $V=3375$, and an image size of $N_{o}=9$, i.e., $V_{o}=729$ with $\sigma=4.6$. Only a few shapes were examined, a football shaped object with a density that increased towards its center, and an anti-football consisting of a rectangular object with a football cut out of its center. No noise was added to the object. These objects were sufficiently small and simple that there was no indication of locking into a local minima.

The data was input for $\sim 10$ patterns in $\vec{k}_{\perp}$ calculated from the input object density distribution at known orientations. The program ran at a rate of $\sim 10$ iterations per minute. The initial image was assumed to be either a constant or random. The constant initial start converged faster than the random start and the results below are for this case. After 15 iterations, the fractional RMS error in the density was typically

$$
\begin{array}{rll}
\sqrt{\left\langle\left(v_{\text {exact }}-v\right)^{2}\right\rangle} /\langle v\rangle & \sim 0.03 & \\
& \sim 0.10 & (\text { anti }- \text { football })  \tag{29}\\
& \sim \text { football })
\end{array}
$$

where $\left\rangle\right.$ indicates an average over the volume $V_{o}$. For 45 iterations, the error ratio for the football dropped to $\sim 0.04$.

One of the advantages of this approach is that the fit to the data does not require any explicit interpolation. Rather, it is performed implicitly by the formalism, see Eq. [5]. One related disadvantage is that the formulation does not admit the simple use of fast fourier transforms to spend up the algorithm. However it should be noted that a full 3-D iteration of the phase iteration method requires the transforms of $N^{3}$ lattice points in addition to the interpolation stage. The Hamiltonian method here requires the transform of $M \times N^{2}$ lattice points. Normally, one expects that $M$ is considerably smaller than $N$. A test of the method on realistic data and a comparison with other methods is planned.

## ACKNOWLEDGEMENTS

I wish to thank Dr. Jianwei Miao, who patiently introduced me to this subject, and Professors Sidney Drell and Richard Haymaker for several helpful discussions.

## Appendix A-Definition of Transforms

A real positive image sequence $v_{i}$ will be defined by the pixel intensities at a set of discrete 3D points $\vec{r}_{i}=\left(i_{x}, i_{y}, i_{z}\right) \Delta$ with $N$ points in each dimension. Each component is in the range $-I<=i<=I$, where $N=2 I+1$ and for simplicity, the image is thought of as being centered near the origin, $i \approx 0$. This real image, $v_{i}$, can be extended to a complex image with the ultimate requirement that its imaginary part, $w_{i}$, vanishes for the problems of interest in this note. In the applications discussed in the text, the spatial integrals extend only over the restricted smaller volume $V_{o}$, since the density vanishes identically in the outer region.

The fourier transform used here is given by

$$
\begin{equation*}
F[k]=\sum_{j}\left(v_{j}+i w_{j}\right) \exp [-i \chi(j, k)], \tag{30}
\end{equation*}
$$

where all sums are over 3-D lattices, i.e., $j=\left(j_{x}, j_{y}, j_{z}\right)$. The inverse is

$$
\begin{align*}
v_{j}+i w_{j} & =\frac{1}{V_{3}} \sum_{k} F[k] \exp [+i \chi(j, k)],  \tag{31}\\
\text { where } \quad \chi(j, k) & =K_{0}\left[j_{x} k_{x}+j_{y} k_{y}+j_{z} k_{z}\right] \tag{32}
\end{align*}
$$

with $K_{0}=2 \pi / N$ and $V_{3}=N^{3}$. It is assumed that the image has support only in the center of the range. Since all the sums in the following discussion are over the fixed interval $-I,-I+$ $1, \ldots, 0, \ldots, I$, only the summation variable will be denoted.

For later use, note the obvious relation

$$
\begin{aligned}
v_{i}+i w_{i} & =\sum_{k} F[k] \exp [+i \chi(i, k)]=\frac{1}{V_{3}} \sum_{k} \sum_{j}\left(v_{j}+i w_{j}\right) \exp \left[+i k_{1}(i-j) k\right] \\
& =\sum_{j}\left(v_{j}+i w_{j}\right) \delta(i, j)=v_{j}+i w_{j}
\end{aligned}
$$

where $\delta(i, j)$ is the Kronecker delta function. Recall the normalization condition

$$
\begin{equation*}
\sum_{k}|F[k]|^{2}=V_{3} \sum_{j}\left(v_{j}^{2}+w_{j}^{2}\right) . \tag{33}
\end{equation*}
$$

Now introduce the magnitude and phase of the transform as

$$
\begin{equation*}
F[\vec{k}]=M[\vec{k}] \exp [-i \phi[\vec{k}]] \tag{34}
\end{equation*}
$$

Equations (30) and (31) can now be written as the pairs

$$
\begin{align*}
M[\vec{k}] \cos \phi[\vec{k}] & =\sum_{j}\left[v_{j} \cos \chi(j, k)+w_{j} \sin \chi(j, k)\right] \\
M[\vec{k}] \sin \phi[\vec{k}] & =\sum_{j}\left[v_{j} \sin \chi(j, k)-w_{j} \cos \chi(j, k)\right]  \tag{35}\\
v_{i} & =\frac{1}{V_{3}} \sum_{k} M[\vec{k}][\cos \phi[\vec{k}] \cos \chi(i, k)+\sin \phi[\vec{k}] \sin \chi(i, k)] \\
w_{i} & =\frac{1}{V_{3}} \sum_{k} M[\vec{k}][\cos \phi[\vec{k}] \sin \chi(i, k)-\sin \phi[\vec{k}] \cos \chi(i, k)] \tag{36}
\end{align*}
$$

We will deal with the two variables $\cos \phi[\vec{k}]$ and $\sin \phi[\vec{k}]$ since this simplifies the choice of branch for the angle $\phi[\vec{k}]$.

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[12] A perhaps more familiar way to implement this requirement is to add a term to the energy that is positive if the image pixel goes negative, such as $\lambda_{j}=\lambda \Theta\left(-v_{j}\right)$. $\lambda$ is then increased as the iteration proceeds. This scheme may allow the system to achieve a lower energy value since it permits the parameters to pass through both the allowed and the ultimately forbidden regions for $v[\vec{r}]$. It is clear that this method functions similarly to the Lagrange inequality multiplier approach.
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[^0]:    ${ }^{1}$ Work supported by the Department of Energy, contract DE-AC03-76SF00515.
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