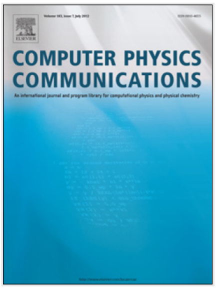

# A tractable prescription for large-scale free flight expansion of wavefunctions

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PII: S0010-4655(16)30234-X
DOI: http://dx.doi.org/10.1016/j.cpc.2016.08.004
Reference: COMPHY 6020

To appear in: *Computer Physics Communications*

Received date: 10 February 2016
Revised date: 6 July 2016
Accepted date: 6 August 2016

Please cite this article as: P. Deuar, A tractable prescription for large-scale free flight expansion of wavefunctions, *Computer Physics Communications* (2016), http://dx.doi.org/10.1016/j.cpc.2016.08.004

# A tractable prescription for large-scale free flight expansion of wavefunctions

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## Abstract

A numerical recipe is given for obtaining the density image of an initially compact quantum mechanical wavefunction that has expanded by a large but finite factor under free flight. The recipe given avoids the memory storage problems that plague this type of calculation by reducing the problem to the sum of a number of fast Fourier transforms carried out on the relatively small initial lattice. The final expanded state is given exactly on a coarser magnified grid with the same number of points as the initial state. An important application of this technique is the simulation of measured time-of-flight images in ultracold atom experiments, especially when the initial clouds contain superfluid defects. It is shown that such a finite-time expansion, rather than a far-field approximation is essential to correctly predict images of defect-laden clouds, even for long flight times. Examples shown are: an expanding quasicondensate with soliton defects and a matter-wave interferometer in 3D.

*Keywords:* Discrete Fourier transform, Ultracold atoms, Free flight evolution, Time of flight imaging, Far-field image, Solitons, Wavefunction, Classical field,
*PACS:* 02.60.Cb, 02.70.-c, 67.85.-d, 03.75.Lm, 03.75.-b

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## 1. Introduction

The free flight expansion of a quantum wavefunction, though physically very simple, is often a troublesome computational problem if the state that is required is not quite yet in the far field regime. The snag is that a computational lattice that both resolves the small initial cloud and encompasses the large expanded cloud can be prohibitively large. Here, it will be described how to overcome this while still using standard discrete fast Fourier transform (FFT) tools.

For example, this is commonly desired when simulating experiments in ultracold atoms. A ubiquitous experimental procedure in this field is the release of the atoms from a trap and the subsequent observation of the density of a strongly expanded cloud. Given that the imaged expanded cloud is usually much larger than the initial one pre-release, the observed expanded atom density corresponds approximately to the velocity distribution in the initial cloud. More precisely, it corresponds to the velocity distribution that is formed early on after release, when the interatomic interaction energy has been converted into kinetic energy. This is the picture that is often used to interpret the data.

This interpretation assumes that the detection is occurring in the far field where all structure is large compared to the initial cloud. However, in practice this is often not a good enough approximation, particularly if one is interested in fine structure inside the atomic cloud, such as defects or interparticle correlations. The reality is that the expansion is usually by a factor of tens or hundreds, so that interesting features such as defects or correlations that are of the order of 10% or 1% of the initial cloud in size have not yet yet attained a velocity profile at the time of detection. They are already distorted from their spatial profile in the initial cloud, but their shape has not yet stabilized to its far field form. Some examples where a long but not quite far-field expansion occurs include the interference pattern generated after release of a pair of elongated clouds [1, 2], the study of Hanbury Brown-Twiss correlations in expanding clouds [3, 4] and two-particle correlations in a halo of supersonically scattered atoms [5, 6].

The basic numerical task here is to predict the detected density image based on whatever model we are using for the atomic field. For excited or thermal gases an ensemble of classical field [7–13] or truncated Wigner wavefunctions

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*Preprint submitted to Elsevier* *July 6, 2016*