Notes – scaling for expansion of atomic clouds

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A. Mod-arg

The GPE is

$$\hbar\frac{\partial\psi(\mathbf{x})}{\partial t} = -i\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + g|\psi(\mathbf{x})|^2\right]\psi(\mathbf{x}). \quad (1)$$

If we consider time-of-flight expansion, this equation when treated using a complex field ψ quickly becomes inconvenient because velocity (roughly constant at long times) is encoded in the phase modulation, with a constant wavelength, while the size of the system grows. This needs ever more lattice points.

However, the field can be rewritten in terms of mod and arg, through

$$\psi(\mathbf{x}) = r(\mathbf{x})e^{i\theta(\mathbf{x})}. \quad (2)$$

From physical arguments we know that as it expands, the relevant length-scales for the density envelope r and the (unrectified) phase θ in the gas will generally grow accordingly. Just that the gradient of θ will tend to stay constant, leading to ever greater values as one travels away from the center. However, if we remain with the phase θ, large values $\gg 2\pi$ do not pose a fundamental problem.

The GPE in these variables becomes

$$\hbar\frac{\partial r(\mathbf{x})}{\partial t} = -\frac{\hbar^2}{2m}\left[r(\mathbf{x})\nabla^2\theta(\mathbf{x}) + 2\nabla r(\mathbf{x})\cdot\nabla\theta(\mathbf{x})\right] \quad (3a)$$

$$\hbar\frac{\partial\theta(\mathbf{x})}{\partial t} = -\left[V(\mathbf{x}) + gr(\mathbf{x})^2\right] + \frac{\hbar^2}{2m}\left[\frac{1}{r(\mathbf{x})}\nabla^2 r(\mathbf{x}) - \nabla\theta(\mathbf{x})\cdot\nabla\theta(\mathbf{x})\right] \quad (3b)$$

Here, the first equation and the last term of the second equation correspond to compressionless hydrodynamics (with $v(\mathbf{x}) = (\hbar/m)\nabla\theta(\mathbf{x})$ and current $j(\mathbf{x}) = r(\mathbf{x})^2 v(\mathbf{x})$). The first line of the $d\theta/dt$ equation gives the (nonlinear) potential for the gas. The first term in the last line is the celebrated and inconvenient quantum pressure term.

It is inconvenient because of the $1/r$ divergence which becomes onerous near nodes of the field. These typically occur around defects such as solitons and vortices, which is troublesome because the point of setting up these equations will be to deal with exactly such defects during expansion.

B. Expansion rate scaling

Let us scale the coordinates as

$$\mathbf{x} = \lambda(t)\cdot\mathbf{z} \quad (4)$$

with $\mathbf{z}$ being the new space variables, and scaling factors λ_j in the jth dimension. It is convenient to allow for different expansion rates in the different directions. Let us assume linear expansion of the coordinates and box via

$$\lambda_j = 1 + c_j t, \quad (5)$$

such that at $t = 0$ there is no scaling and $x_j + z_j$. It can be notationally convenient to define inverse scaling factors

$$\varepsilon_j(t) = \frac{1}{\lambda_j} \leqslant 1. \quad (6)$$

Then e.g. $\mathbf{z} = \varepsilon\cdot\mathbf{x}$.

Further, let us keep the wavefunction normalized, so that if the wavefunction in the scaled coordinates is $\phi(\mathbf{z})$, then

$$N = \int d^d\mathbf{x}|\psi(\mathbf{x})|^2 = \int d^d\mathbf{z}|\phi(\mathbf{z})|^2. \quad (7)$$

This leads immediately to

$$\phi(\mathbf{z}) = \psi(\mathbf{x})\sqrt{\Pi_j\lambda_j}. \quad (8)$$

In mod-arg variables

$$\phi(\mathbf{z}) = R(\mathbf{z})e^{i\theta(\mathbf{z})} \quad (9)$$

this becomes

$$R(\mathbf{z}) = r(\mathbf{x})\sqrt{\Pi_j\lambda_j}. \quad (10)$$

The phase θ is unaffected. Note that the scaling factors are time-dependent.

Processing the variable change, one arrives at the following equations:

$$\hbar\frac{\partial R(\mathbf{z})}{\partial t} = -\frac{\hbar^2}{2m}\sum_j \varepsilon_j^2(t)\left[R(\mathbf{z})\frac{\partial^2\theta(\mathbf{z})}{\partial z_j^2} + 2\frac{\partial R(\mathbf{z})}{\partial z_j}\,\frac{\partial\theta(\mathbf{z})}{\partial z_j}\right] + \sum_j \frac{c_j\varepsilon_j}{2}\,R(\mathbf{z}) \tag{11a}$$

$$\hbar\frac{\partial\theta(\mathbf{x})}{\partial t} = -\left[V(\mathbf{z}) + gR(\mathbf{z})^2\ (\Pi_j\varepsilon_j)\right] + \frac{\hbar^2}{2m}\sum_j \varepsilon_j^2\left[\frac{1}{R(\mathbf{z})}\frac{\partial^2 R(\mathbf{z})}{\partial z_j^2} - \frac{\partial\theta(\mathbf{z})}{\partial z_j}\,\frac{\partial\theta(\mathbf{z})}{\partial z_j}\right] \tag{11b}$$

with ∇ now referring to gradient with respect to $\mathbf{z}$. these can be kept on the same numerical lattice as initially, with one possible and important caveat:

C. Cut-outs

So trouble brews if the quantum pressure term hits a zero. Here is a possible solution:

First, we should realize that (I hope) this is a relatively rare occurence. Further, it is likely that the number of defects stays approx constant as evolution proceeds. The idea then would be to locate the divergent spots, cut out a piece of space there, and evolve it according to the standard complex GPE. The difficulty is that as time proceeds, we will have a phase jump of more than 2π over primary lattice points there, so that the wavefunction will be aliased, and therefore "kicha". We can try to assume, though, that the phase and density gradient there is smooth. So the thing to do would be to make an interpolating sub-lattice and evolve on that.

First question: when is a spot bad enough to treat specially? Certainly, if $1/R$ varies by more than R over a lattice spacing Δz_j, then it is bad. In fact, we don't want to let it even approach that because a minumum might be missed since $R \geqslant 0$ always. Suppose the following condition: Lattice point $\mathbf{z}$ is suspect if

$$\frac{R(\mathbf{z} + \hat{e}_\nu \cdot \Delta\mathbf{z})}{R(\mathbf{z})} > 1 + s. \tag{12}$$

where $\hat{e}_\nu$ are positive and negative unit vectors used to indicate neighbouring points on the lattice, and s is a numerical parameter to be chosen. As s is reduced, more suspect points are identified. By eye, a value of $s = 0.5$ might be good. Note that $R(\mathbf{z}) \geqslant 0$ always, so the left hand side is always positive. If this LHS is less than one, it means that the neighbouring point is the lower and more suspect one, so we can move on.

The proposed algorithm for each time step is then like this:

1. Calculate $d\theta(\mathbf{z})/dt$ and $dR(\mathbf{z})/dt$ for the whole field.
2. Identify any suspect points using (12).
3. For each suspect point $\mathbf{y}$, carry out a little sub-calculation of these derivatives on a finer lattice, pick out the resulting value at the original lattice point, and substitute it instead of the coarse-grained value obtained in point 1. above.
4. Use the augmented derivative (with substitutions) to evolve R and θ on the usual coarse lattice.

The sub-calculation for a point $\mathbf{y}$ would look like this:

1. Find the phase jump between left/right neighbours of the point $\mathbf{y}$; Call it $\Delta\Theta_j$ (one for each dimension).
2. To be sensible, the fine calculation cannot have more than about $\pi/2$ phase jump over any lattice point. Hence, the number of points in that dimension should be $\geqslant 1 + \Delta\Theta_j/(\pi/2)$. In practice, it would be useful to have at least twice this density, and to cap it from below to 8 or something like that.
3. We set up the new lattice $\overline{\mathbf{z}}$, and interpolate θ and R values over it (linearly, as a first guess). Then convert this explicitly to a complex wavefunction $\phi(\overline{\mathbf{z}})$.
4. Calculate the time derivative of this fine wavefunction with the (scaled) GPE:

$$\hbar\frac{\partial\phi(\mathbf{z})}{\partial t} = \left[i\frac{\hbar^2}{2m}\sum_j \varepsilon_j^2\frac{\partial^2}{\partial z_j^2} - iV(\mathbf{z}) - ig|\phi(\mathbf{z})|^2(\Pi_j\varepsilon_j) + \frac{\sum_j c_j\varepsilon_j}{2}\right]\phi(\mathbf{z}) \tag{13}$$

   This can probably be done analytically, actually, without resorting to the fine lattice. Work on that!
5. Pick the derivative at the central point and amend the global derivative at $\mathbf{y}$ on the $\mathbf{x}$ lattice accordingly.

A better version of this algorithm would use not just the nearest neighbours, for interpolation, but some kind of maybe parabolic or spline fit using the next-nearest neighbours of $\mathbf{y}$.

D. Extensions

This is in some ways both better and worse than the previously published discrete black-box algorithm [1]:

- Better: Does not explicitly cut the interaction out sharply after some time, but keeps it in fully all the way.
- Better: Numerical effort here scales as number of timesteps: $\sim t$, as opposed to $\sim \lambda^d\, t^d$ in the black-box. It is better then, in this regard, for 2d and 3d. NOTE: That's without the extra cut-out bits. With those, it depends on whether an analytical solution is provided in the end or not, but any scaling with t here will only kick in significantly for pretty big expansion.
- Worse: The quantum pressure terms causes trouble here, but was no problem for the black-box algorithm. How much trouble remains to be seen, and is a major subject of the proposed paper.

The basic equation is probably not a huge revelation (mostly hydrodynamic equations?) However, among other points we wish to present here are extensions to cases with: dipolar or other ranged interactions, positive-P STAB type terms, ...

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[1] P. Deuar Comput. Phys. Commun. **208**, 92 (2016).