I. EQUATIONS OF MOTION

The Schrodinger-Poisson system is a Schrodinger equation whose potential solves a Poisson equation as follows:

$$i\Psi_t = -\frac{1}{2}\Delta\Psi + gV\Psi \tag{1}$$
$$\Delta V = \Psi\Psi^* \tag{2}$$

, where g is a coupling constant.
Using the form of the laplacian in spherical symmetry, the Poisson equation becomes:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial V}{\partial r}\right) = \Psi\Psi^* \tag{3}$$

II. SCALING

The size of the coupling constant g depends on the normalization of the wavefunction. In our code, the initial wavefunction can be initialized with arbitrary normalization, but in the computation the wavefunctions are renormalized with unit norm so that the size of g does not depend on the choice of initialization.

III. BOUNDARY CONDITIONS

Smoothness at the origin is better enforced by the numerical scheme if the differential operator is rewritten in terms of r^3,

$$\Delta V = 3\frac{\partial}{\partial r^3}\left(r^2\frac{\partial V}{\partial r}\right) \tag{4}$$

To simplify things, we impose that all functions are zero at a finite outer boundary r = 1,

$$V|_{r=1} = 0 \tag{5}$$
$$\Psi|_{r=1} = 0 \tag{6}$$

and are smooth at the origin,

$$\frac{dV}{dr}|_{r=0} = 0 \tag{7}$$
$$\frac{d\Psi}{dr}|_{r=0} = 0 \tag{8}$$

IV. DISCRETIZATION

To discretize the spatial domain into Nx grid points, FORTRAN notation is used, ie:

$$r_1 = 0 \tag{9}$$
$$r_2 = h \tag{10}$$
$$r_3 = 2h \tag{11}$$
$$\vdots \tag{12}$$
$$r_{\mathrm{Nx}} = 1 \tag{13}$$

By introducing the $\mathcal{O}(h^2)$ accurate forward-differencing derivative operator,

$$(f_{\mathrm{x}})_j^n = \frac{-\frac{3}{2}f_j^n + 2f_{j+1}^n - \frac{1}{2}f_{j+2}^n}{h} + \mathcal{O}(h^2) \tag{14}$$

The inner boundary condition becomes:

$$f_1^n = -\frac{1}{3}f_3^n + \frac{4}{3}f_2^n \tag{15}$$

where f is either V or Ψ. This allows for all references to V_1 and Ψ_1 to be removed from the the finite-differencing scheme.

In order to discretize the Laplacian as written in equation 4 as $\mathcal{O}(h^2)$ centred at r_j, it is necessary to introduce "half spatial points":

$$r_{j+\frac{1}{2}} \equiv r_j + \frac{dr}{2} \tag{16}$$

$$r_{j-\frac{1}{2}} \equiv r_j - \frac{dr}{2} \tag{17}$$

then

$$\Delta f = \frac{3}{r_{j+\frac{1}{2}}^3 - r_{j-\frac{1}{2}}^3}\left(r_{j+\frac{1}{2}}^2 * \left(\frac{f_{j+1} - f_j}{dr}\right) - r_{j-\frac{1}{2}}^2 * \left(\frac{f_j - f_{j-1}}{dr}\right)\right) \tag{18}$$

V. TRIDIAGONAL FORM

Using the above discretization for the laplacian, the Poisson equation for V can be written in tridiagonal form:

$$c_- V_{j-1} + c_0 V_j + c_+ V_{j+1} = \Psi_j \Psi_j^* \tag{19}$$

where

$$c_- = \frac{3}{dr}\left(\frac{r_{j-\frac{1}{2}}^2}{r_{j+\frac{1}{2}}^3 - r_{j-\frac{1}{2}}^3}\right) \tag{20}$$

$$c_0 = -\frac{3}{dr}\left(\frac{r_{j-\frac{1}{2}}^2 + r_{j+\frac{1}{2}}^2}{r_{j+\frac{1}{2}}^3 - r_{j-\frac{1}{2}}^3}\right) \tag{21}$$

$$c_+ = \frac{3}{dr}\left(\frac{r_{j+\frac{1}{2}}^2}{r_{j+\frac{1}{2}}^3 - r_{j-\frac{1}{2}}^3}\right) \tag{22}$$

And the reference to V_1 in equation 19 can be eliminated using equation 15:

$$c_-\left(\frac{4}{3}V_2^n - \frac{1}{3}V_3^n\right) + c_0 V_2 + c_+ V_3 = \Psi_2 \Psi_2^* \tag{23}$$

and so the first row entries of the tridiagonal matrix describing the discretized Poisson equation are given by

$$\frac{4}{3}c_- + c_0 = \frac{1}{dr}\left(\frac{r_{2-\frac{1}{2}}^2 - 3r_{2+\frac{1}{2}}^2}{r_{2+\frac{1}{2}}^3 - r_{2-\frac{1}{2}}^3}\right) \tag{24}$$

$$c_+ - \frac{1}{3}c_- = \frac{1}{dr}\left(\frac{3r_{2+\frac{1}{2}}^2 - r_{2-\frac{1}{2}}^2}{r_{2+\frac{1}{2}}^3 - r_{2-\frac{1}{2}}^3}\right) \tag{25}$$

For the Schrodinger equation we apply a forward-difference time derivative operator to the left hand side which is $\mathcal{O}(h^2)$ accurate at $t_{n+\frac{1}{2}}$. To center the rest of the equation at time $t_{n+\frac{1}{2}}$ we appy the forward-time averaging operator,μ, to the right hand side. This gives:

$$i\frac{\Psi_j^{n+1} - \Psi_j^n}{dt} = -\frac{1}{2}\mu\Delta\Psi + \mu g V \Psi \tag{26}$$

Treating the retarded and advanced time levels of V as known, and using our discretization of the Laplacian this can be brought into tridiagonal form:

$$d_-\Psi_{j-1} + d_0\Psi_j + d_+\Psi_{j+1} = F(j) \tag{27}$$

where

$$d_- = \frac{3}{4}\frac{dt}{dr}\left(\frac{r^2_{j-\frac{1}{2}}}{r^3_{j+\frac{1}{2}} - r^3_{j-\frac{1}{2}}}\right) \tag{28}$$

$$d_0 = i - \frac{3}{4}\frac{dt}{dr}\left(\frac{r^2_{j-\frac{1}{2}} + r^2_{j+\frac{1}{2}}}{r^3_{j+\frac{1}{2}} - r^3_{j-\frac{1}{2}}}\right) - \frac{dt}{2}gV_j^{n+1} \tag{29}$$

$$d_+ = \frac{3}{4}\frac{dt}{dr}\left(\frac{r^2_{j+\frac{1}{2}}}{r^3_{j+\frac{1}{2}} - r^3_{j-\frac{1}{2}}}\right) \tag{30}$$

$$F(j) = i\Psi_j^n - \frac{3}{4}\frac{dt}{dr}\left(\frac{r^2_{j+\frac{1}{2}}\left(\Psi^n_{j+1} - \Psi^n_j\right) - r^2_{j-\frac{1}{2}}\left(\Psi^n_j - \Psi^n_{j-1}\right)}{r^3_{j+\frac{1}{2}} - r^3_{j-\frac{1}{2}}}\right) + \frac{dt}{2}gV_j^n\Psi_j^n \tag{31}$$

Where again Ψ_1 can be eliminated using equation 15:

$$d_-\left(\frac{4}{3}\Psi_2^n - \frac{1}{3}\Psi_3^n\right) + d_0\Psi_2 + d_+\Psi_3 = F(2) \tag{32}$$

And so the entries of the first row of the tridiagonal matrix which defines the Schrodinger equation are given by:

$$\frac{4}{3}d_- + d_0 = i + \frac{1}{4}\frac{dt}{dr}\left(\frac{r^2_{2-\frac{1}{2}} - 3r^2_{2+\frac{1}{2}}}{r^3_{2+\frac{1}{2}} - r^3_{2-\frac{1}{2}}}\right) - \frac{dt}{2}gV_2^{n+1} \tag{33}$$

$$d_+ - \frac{1}{3}d_- = \frac{1}{4}\frac{dt}{dr}\left(\frac{3r^2_{2+\frac{1}{2}} - r^2_{2-\frac{1}{2}}}{r^3_{2+\frac{1}{2}} - r^3_{2-\frac{1}{2}}}\right) \tag{34}$$

VI. NORM CALCULATION

The norm of the wavefunction, Ψ, in spherical symmetry is,

$$I(r) = 4\pi\int_0^r \xi^2|\Psi(\xi)|^2\,d\xi \tag{35}$$

The value of I at the outer boundary should be nearly conserved, and exactly conserved if $V = 0$. To calculate this integral numerically we employ a Riemann sum using the midpoint rule,

$$I(r_j) = I(r_{j-1}) + dr\left(r(j) - \frac{dr}{2}\right)^2\frac{(\Psi_j + \Psi_{j-1})}{2}\frac{\left(\Psi^*_j + \Psi^*_{j-1}\right)}{2} \tag{36}$$

and $I(r_1) \equiv 0$. Notice we have excluded the factor of 4π since we are only concerned with how well the value of I at the outer boundary is conserved.

VII. INDEPENDENT RESIDUAL CALCULATION

To check that the code is really producing solutions to the finite difference equations (Eqs. 27 - 31) we use an alternative finite difference scheme given by

$$\tilde{L}[\tilde{\Psi}] = 0 \tag{37}$$

and then apply $\tilde{L}$ to the solution of the original finite difference scheme, Ψ. If the code is actually producing solutions to the finite differencing scheme of interest, then we should find that

$$\lim_{dr\to 0} \tilde{L}[\Psi] = 0 \tag{38}$$

For the alternative finite difference scheme, we no longer use the half-time level and use a Leap Frog scheme, such that the $\mathcal{O}(dt^2)$ accurate centered time derivative is now approximated by,

$$\frac{\Psi_j^{n+1} - \Psi_j^{n-1}}{2dt} = \frac{\partial \Psi_j^n}{\partial t} + \mathcal{O}(dt^2) \tag{39}$$

The operator $\tilde{L}$ is given by

$$\tilde{L}[\Psi_j^n] = \quad i\frac{\left(\Psi_j^{n+1} - \Psi_j^{n-1}\right)}{2dt} \tag{40}$$

$$+ \quad \frac{3}{2dr}\frac{r_{j+\frac{1}{2}}^2\left(\Psi_{j+1}^n - \Psi_j^n\right) - r_{j-\frac{1}{2}}^2\left(\Psi_j^n - \Psi_{j-1}^n\right)}{r_{j+\frac{1}{2}}^3 - r_{j-\frac{1}{2}}^3} \tag{41}$$

$$- \quad gV_j^n\Psi_j^n \tag{42}$$

The updates thus far have only depended on two time levels, Ψ^n and Ψ^{n+1}, but to implement this alternative mesh convergence test three time levels are required. To deal with this in our code, we introduce a grid function $\Psi_{\rm aux}^{n+1} = \Psi^n$. In this way Ψ^n will be available at the next time step as $\Psi_{\rm aux}^n$. We choose to initialize $\Psi_{\rm aux}^1 = \Psi^1$, but this is false data and so the first time level of the alternative mesh residual is also expected to be false.

VIII. CHANGE OF VARIABLES

To accomodate change of space and time variables, we introduce the new variables in the updates0.inc file. In this way, all grid functions come back to RNPL in the new variables. This means that grid functions that are auto initialized in RNPL have to be initialized in the new variables.

For example, to implement logarithmic space and time variables we make the definitions:

$$r2(j) = ln(1 + r(j)) \tag{43}$$

$$dr2(j) = \frac{dr}{1 + r(j)} \tag{44}$$

$$t2 = ln(1 + t) \tag{45}$$

$$dt2 = \frac{dt}{1 + t} \tag{46}$$

and then replace all previous instances of r,dr,t,dt with r2,dr2,t2,dt2.

One point to be careful of is that the finite difference equations involve half spatial points $r_{j+\frac{1}{2}} = \frac{r_{j+1}+r_j}{2}$. The change of variables in this case carries $r_{j+\frac{1}{2}}$ to

$$r2_{j+\frac{1}{2}} = ln(1 + r_{j+\frac{1}{2}}) \tag{47}$$

which we would not get by blindly replacing all r's with $r2$'s. Fortunately in our code the $r_{j+\frac{1}{2}}$ points are defined by a new variable, and so we can replace all r with $r2$ and all $r_{j+\frac{1}{2}}$ with $r2_{j+\frac{1}{2}}$.

Because RNPL has defined rectangular coordinates r and t, the solutions will be sent to XVS with r and t, and it is understood that the displayed values need to be converted.