The Expression:

$$\frac{-1}{2\,\mu}\,(\text{Laplacian}[\psi[\text{r1},\text{r2},\text{t}],\{\text{r1},\text{r2}\}]) - Z\,(e^{\wedge}2)\left(\frac{1}{\text{r1}}+\frac{1}{\text{r2}}\right) - \frac{1}{M}\,(\text{grad1.grad2}) + \frac{(e^{\wedge}2)}{\text{r12}}$$

Look at lattice expressions of the Helium quantum wavefunction because I found that it gives an interesting example of symmetry and broken symmetry, the types we more commonly use (basically resort to) in particle physics. Very interesting to see such phenomena at the level of quantum physics where the concepts are a bit more tractable, typically we're just shoveled these concepts while studying particle physics. Explain this symmetry and broken symmetry in the green box.

Otherwise designed to be helpful for those seeking to implement quantum wave functions, or lattice appxs of them, on computer algebra or standard coding frameworks.

Some Basics and Individual Partial Derivatives (See if you're having trouble managing the full expression)

```
Laplacian[ψ[x1, y1, z1, x2, y2, z2, t], {x1, y1, z1}]
Laplacian[ψ[x1, y1, z1, x2, y2, z2, t], {x2, y2, z2}]
Laplacian[ψ[x1, y1, z1, x2, y2, z2, t], {x1, y1, z1, x2, y2, z2}]

Laplacian[ψ[r1, r2, t], {r1, r2}]
(Laplacian[ψ[r1, r2, t], {r1}] + Laplacian[ψ[r1, r2, t], {r2}] )
(*Same as doing just Laplacian[ψ[r1,r2,t],{r1,r2}] *)
```

$\psi^{(0,0,2,0,0,0,0)}[\text{x1, y1, z1, x2, y2, z2, t}] + \psi^{(0,2,0,0,0,0,0)}[\text{x1, y1, z1, x2, y2, z2, t}] + \psi^{(2,0,0,0,0,0,0)}[\text{x1, y1, z1, x2, y2, z2, t}]$

$\psi^{(0,0,0,0,0,2,0)}[\text{x1, y1, z1, x2, y2, z2, t}] + \psi^{(0,0,0,0,2,0,0)}[\text{x1, y1, z1, x2, y2, z2, t}] + \psi^{(0,0,0,2,0,0,0)}[\text{x1, y1, z1, x2, y2, z2, t}]$

$\psi^{(0,0,0,0,0,2,0)}[\text{x1, y1, z1, x2, y2, z2, t}] + \psi^{(0,0,0,0,2,0,0)}[\text{x1, y1, z1, x2, y2, z2, t}] + \psi^{(0,0,0,2,0,0,0)}[\text{x1, y1, z1, x2, y2, z2, t}] + \psi^{(0,0,2,0,0,0,0)}[\text{x1, y1, z1, x2, y2, z2, t}] + \psi^{(0,2,0,0,0,0,0)}[\text{x1, y1, z1, x2, y2, z2, t}] + \psi^{(2,0,0,0,0,0,0)}[\text{x1, y1, z1, x2, y2, z2, t}]$

$\psi^{(0,2,0)}[\text{r1, r2, t}] + \psi^{(2,0,0)}[\text{r1, r2, t}]$

$\psi^{(0,2,0)}[\text{r1, r2, t}] + \psi^{(2,0,0)}[\text{r1, r2, t}]$

```
Grad[ψ[r1, r2, t], {r1}]
Grad[ψ[r1, r2, t], {r2}]
ψ[x1, y1, z1, x2, y2, z2, t]
grad12 = D[ψ[x1, y1, z1, x2, y2, z2, t], x1, x2] +
  D[ψ[x1, y1, z1, x2, y2, z2, t], y1, y2] + D[ψ[x1, y1, z1, x2, y2, z2, t], z1, z2]
```

$\{\psi^{(1,0,0)}[r1, r2, t]\}$

$\{\psi^{(0,1,0)}[r1, r2, t]\}$

$\psi[x1, y1, z1, x2, y2, z2, t]$

$$\psi^{(0,0,1,0,0,1,0)}[x1, y1, z1, x2, y2, z2, t] + \psi^{(0,1,0,0,1,0,0)}[x1, y1, z1, x2, y2, z2, t] + \psi^{(1,0,0,1,0,0,0)}[x1, y1, z1, x2, y2, z2, t]$$

$\sqrt{x1^2 + y1^2 + z1^2}$ (* = r1 *)

$\sqrt{x2^2 + y2^2 + z2^2}$ (* = r2 *)

$\sqrt{(x1 - x2)^2 + (y1 - y2)^2 + (z1 - z2)^2}$ (* = r12 *)

Full Computer Algebra Expression

$$\frac{-1}{2\mu}\left(\text{Laplacian}[\psi[x1, y1, z1, x2, y2, z2, t], \{x1, y1, z1, x2, y2, z2\}]\right) - \left(Z\,(e\hat{}2)\left(\frac{1}{\sqrt{x1^2 + y1^2 + z1^2}} + \frac{1}{\sqrt{x2^2 + y2^2 + z2^2}}\right)\psi[x1, y1, z1, x2, y2, z2, t]\right) - \left(\frac{1}{M}\,(\text{grad12})\right) + \frac{(e\hat{}2)}{\sqrt{(x1 - x2)^2 + (y1 - y2)^2 + (z1 - z2)^2}}\psi[x1, y1, z1, x2, y2, z2, t]$$

$$\frac{e^2\,\psi[x1, y1, z1, x2, y2, z2, t]}{\sqrt{(x1 - x2)^2 + (y1 - y2)^2 + (z1 - z2)^2}} - e^2 Z\left(\frac{1}{\sqrt{x1^2 + y1^2 + z1^2}} + \frac{1}{\sqrt{x2^2 + y2^2 + z2^2}}\right)\psi[x1, y1, z1, x2, y2, z2, t] - \frac{1}{M}\left(\psi^{(0,0,1,0,0,1,0)}[x1, y1, z1, x2, y2, z2, t] + \psi^{(0,1,0,0,1,0,0)}[x1, y1, z1, x2, y2, z2, t] + \psi^{(1,0,0,1,0,0,0)}[x1, y1, z1, x2, y2, z2, t]\right) - \frac{1}{2\mu}\left(\psi^{(0,0,0,0,0,2,0)}[x1, y1, z1, x2, y2, z2, t] + \psi^{(0,0,0,0,2,0,0)}[x1, y1, z1, x2, y2, z2, t] + \psi^{(0,0,0,2,0,0,0)}[x1, y1, z1, x2, y2, z2, t] + \psi^{(0,0,2,0,0,0,0)}[x1, y1, z1, x2, y2, z2, t] + \psi^{(0,2,0,0,0,0,0)}[x1, y1, z1, x2, y2, z2, t] + \psi^{(2,0,0,0,0,0,0)}[x1, y1, z1, x2, y2, z2, t]\right)$$

Lattice Approximations for dealing with the wavefn numerically

As an explicit example, the mixed partial derivative D[ψ[x1,x2],x1,x2] = $\frac{\partial\psi}{\partial x1\,\partial x2}$ has the lattice appx given in the following cell. For those who don't immediately recall how to get lattice expression in numerical appx of derivatives, simply recall the definition of the derivative as an infinitesimal limit of [f(x + h) - f(x)]/ h, apply limite to the lattice expressions and get derivatives

$$D[\psi[x1, x2], x1, x2] \rightarrow \frac{\psi[x1 + h1, x2 + h2] - \psi[x1 + h1, x2] - \psi[x1, x2 + h2] + \psi[x1, x2]}{(h1\, h2)}$$

$$\frac{-1}{2\mu}\left(\frac{(\psi[x1 + 2\,h1, x2] - \psi[x1 + h1, x2] + \psi[x1, x2])}{h1} + \frac{(\psi[x1, x2 + 2\,h2] - \psi[x1, x2 + h2] + \psi[x1, x2])}{h2}\right) - \left(Z\,(e\hat{}2)\left(\frac{1}{x1} + \frac{1}{x2}\right)\right)(\psi[x1, x2]) - \frac{1}{M}\left(\frac{\psi[x1 + h1, x2 + h2] - \psi[x1 + h1, x2] - \psi[x1, x2 + h2] + \psi[x1, x2]}{(h1\, h2)}\right) + \frac{(e\hat{}2)}{Abs[(x2 - x1)]}\psi[x1, x2]$$

let $h1 = h2 = h,\ x1 = n_1 h,\ x2 = n_2 h$

$$\frac{-1}{2\mu}\left(\frac{(\psi[x1 + 2\,h1, x2] - \psi[x1 + h1, x2] + \psi[x1, x2])}{h1} + \frac{(\psi[x1, x2 + 2\,h2] - \psi[x1, x2 + h2] + \psi[x1, x2])}{h2}\right) - \left(Z\,(e\hat{}2)\left(\frac{1}{x1} + \frac{1}{x2}\right)\right)(\psi[x1, x2]) - \frac{1}{M}\left(\frac{1}{(h1\, h2)}(\psi[x1 + h1, x2 + h2] - \psi[x1 + h1, x2] - \psi[x1, x2 + h2] + \psi[x1, x2])\right) + \frac{(e\hat{}2)}{Abs[(x2 - x1)]}\psi[x1, x2] \;/.\; h1 \to h \;/.\; h2 \to h \;/.\; x1 \to n_1 h \;/.\; x2 \to n_2 h \;//\; Simplify$$

$$\left(\frac{e^2}{Abs[h\,(-n_1 + n_2)]} - \frac{\frac{1}{M} + \frac{h}{\mu} + \frac{e^2 h Z}{n_1} + \frac{e^2 h Z}{n_2}}{h^2}\right)\psi[h\,n_1, h\,n_2] + \frac{1}{2\,h^2 M \mu}$$
$$\left(-h\,M\,\psi[h\,n_1, h\,(2 + n_2)] + (h\,M + 2\mu)\,\psi[h\,n_1, h + h\,n_2] - h\,M\,\psi[h\,(2 + n_1), h\,n_2] + h\,M\,\psi[h + h\,n_1, h\,n_2] + 2\mu\,\psi[h + h\,n_1, h\,n_2] - 2\mu\,\psi[h + h\,n_1, h + h\,n_2]\right)$$

$$\left(\frac{e^2}{\text{Abs}[h\ (-n_1+n_2)]}-\frac{\frac{1}{M}+\frac{h}{\mu}+\frac{e^2 h Z}{n_1}+\frac{e^2 h Z}{n_2}}{h^2}\right)\psi[h\,n_1,\ h\,n_2]+\frac{1}{2\,h^2\,M\,\mu}$$

$$\left(-h\,M\,\psi\left[h\,n_1,\ h\ (2+n_2)\right]+(h\,M+2\,\mu)\ \psi[h\,n_1,\ h+h\,n_2]-h\,M\,\psi\left[h\ (2+n_1),\ h\,n_2\right]+ h\,M\,\psi[h+h\,n_1,\ h\,n_2]+2\,\mu\,\psi[h+h\,n_1,\ h\,n_2]-2\,\mu\,\psi[h+h\,n_1,\ h+h\,n_2]\right)\ /.\ e\to 1$$

$$\left(\frac{1}{\text{Abs}[h\ (-n_1+n_2)]}-\frac{\frac{1}{M}+\frac{h}{\mu}+\frac{h Z}{n_1}+\frac{h Z}{n_2}}{h^2}\right)\psi[h\,n_1,\ h\,n_2]+\frac{1}{2\,h^2\,M\,\mu}$$

$$\left(-h\,M\,\psi\left[h\,n_1,\ h\ (2+n_2)\right]+(h\,M+2\,\mu)\ \psi[h\,n_1,\ h+h\,n_2]-h\,M\,\psi\left[h\ (2+n_1),\ h\,n_2\right]+ h\,M\,\psi[h+h\,n_1,\ h\,n_2]+2\,\mu\,\psi[h+h\,n_1,\ h\,n_2]-2\,\mu\,\psi[h+h\,n_1,\ h+h\,n_2]\right)$$

$$H\,\psi=\left(\frac{1}{\text{Abs}[h\ (-n_1+n_2)]}-\frac{\frac{1}{M}+\frac{h}{\mu}+\frac{h Z}{n_1}+\frac{h Z}{n_2}}{h^2}\right)\psi[h\,n_1,\ h\,n_2]+\frac{1}{2\,h^2\,M\,\mu}$$

$$(-h\,M\,\psi[h\,n_1,\ h\ (2+n_2)]+(h\,M+2\,\mu)\ \psi[h\,n_1,\ h+h\,n_2]-h\,M\,\psi[h\ (2+n_1),\ h\,n_2]+ h\,M\,\psi[h+h\,n_1,\ h\,n_2]+2\,\mu\,\psi[h+h\,n_1,\ h\,n_2]-2\,\mu\,\psi[h+h\,n_1,\ h+h\,n_2])$$

$$=\frac{1}{h}\left(\frac{1}{\text{Abs}[(-n_1+n_2)]}-\left(\frac{1}{hM}+\frac{1}{\mu}+\frac{Z}{n_1}+\frac{Z}{n_2}\right)\right)\psi[h\,n_1,\ h\,n_2]\ +$$

$$\left(-\frac{1}{2\,h\,\mu}\right)\ (\psi[h\,n_1,\ h\ (2+n_2)]+\psi[h\ (2+n_1),\ h\,n_2])\ +$$

$$\left(\frac{1}{2\,h\,\mu}+\frac{1}{h^2\,M}\right)\psi[h\,n_1,\ h\ (1+n_2)]+$$

$$\left(\frac{1}{2\,h\,\mu}+\frac{1}{h^2\,M}\right)\psi[h\ (1+n_1),\ h\,n_2]-\frac{1}{h^2\,M}\psi[h\ (1+n_1),\ h\ (1+n_2)]$$

$$=\frac{1}{h}\left(\left(\frac{1}{\text{Abs}[(-n_1+n_2)]}-\left(\frac{1}{hM}+\frac{1}{\mu}+\frac{Z}{n_1}+\frac{Z}{n_2}\right)\right)\psi[h\,n_1,\ h\,n_2]\ +\right.$$

$$\left(-\frac{1}{2\,\mu}\right)\ (\psi[h\,n_1,\ h\ (2+n_2)]+\psi[h\ (2+n_1),\ h\,n_2])\ +\left(\frac{1}{2\,\mu}+\frac{1}{h\,M}\right)\psi[h\,n_1,\ h\ (1+n_2)]+$$

$$\left.\left(\frac{1}{2\,\mu}+\frac{1}{h\,M}\right)\psi[h\ (1+n_1),\ h\,n_2]-\frac{1}{h\,M}\psi[h\ (1+n_1),\ h\ (1+n_2)]\right)$$

(In the $M\to\infty$ Appx, $\mu\to m$, and we can see that the $\psi[h\ (1+n_1),\ h\ (1+n_2)]$ is the only term entirely removed, i.e. $M\to\infty$ appx removes symmetric single – site pertubation but none of the other terms)

Note that $\psi[h\,n_1,\ h\ (1+n_2)]$ and $\psi[h\ (1+n_1),\ h\,n_2]$, the mixed gradient – derived terms, are non – vanishing in the finite M case, whereas they vanish in the $M\to\infty$ Appx

Then, in the Appx where ψ is relatively resistant to change such that $\psi[h\, n_1, h\, n_2] \sim \psi[h\,(1+n_1), h\, n_2]$ very nearly for all the pertubations, we have that

$$H\psi \approx \left(\left(\frac{1}{\text{Abs}[(-n_1+n_2)]} - \left(\frac{1}{hM}+\frac{1}{\mu}+\frac{Z}{n_1}+\frac{Z}{n_2}\right)\right) + \left(-\frac{1}{2\mu}\right)(2) + \left(\frac{1}{2\mu}+\frac{1}{h\,M}\right) + \left(\frac{1}{2\mu}+\frac{1}{h\,M}\right) - \frac{1}{h\,M}\right)\frac{1}{h}\psi[h\, n_1, h\, n_2]$$

$$= \left(\left(\frac{1}{\text{Abs}[(-n_1+n_2)]} - \left(\frac{1}{hM}+\frac{1}{\mu}+\frac{Z}{n_1}+\frac{Z}{n_2}\right)\right) + \frac{1}{h\,M}\right)\frac{1}{h}\psi[h\, n_1, h\, n_2]$$

$$= \left(\frac{1}{\text{Abs}[(-n_1+n_2)]} - Z\left(\frac{1}{n_1}+\frac{1}{n_2}\right) - \frac{1}{\mu}\right)\frac{1}{h}\psi[h\, n_1, h\, n_2]$$

Let $n_2 = n_1 + L$

$$= \left(\frac{1}{\text{Abs}[L]} - Z\left(\frac{1}{n_1}+\frac{1}{n_1+L}\right) - \frac{1}{\mu}\right)\frac{1}{h}\psi[h\, n_1, h\, n_2]$$

$$= \left(\frac{1}{\text{Abs}[L]} - Z\left(\frac{1}{n_1}+\frac{1}{n_1+L}\right) - \frac{1}{\mu}\right)\frac{1}{h}\psi[h\, n_1, h\,(n_1+L)]$$

And for n1 >> L (electrons near each other on the scale of L) we have that (Can also let $(x2-x1) = h\,L \sim \xi$ the correlation distance)

$$H\psi \approx \left(\frac{1}{\text{Abs}[L]} - Z\left(\frac{2}{n_1}\right) - \frac{1}{\mu}\right)\frac{1}{h}\psi[h\, n_1, h\, n_1]$$

And for $n_1 \sim L$

$$H\psi \approx \left(\frac{1}{L} - Z\left(\frac{3}{2\,L}\right) - \frac{1}{\mu}\right)\frac{1}{h}\psi[h\, L, h\,(2\,L)] =$$

$$\left(\left(1-\frac{3}{2}Z\right)\frac{1}{L} - \frac{1}{\mu}\right)\frac{1}{h}\psi[h\, L, h\,(2\,L)]$$

(* Have broken symmetry term $+\frac{1}{h\,M}$ from same term that goes to 0 in M → ∞ Appx., although interestingly this cancels with another term, so M → ∞ Appx. doesn't fundamentally alter the symmetry in the slowly varying case, Moreover, in the M→ ∞ Appx $-\frac{1}{hM}$ goes to zero anyway even though uncancelled, HOWEVER, simply letting $\psi[h\,(1+n_1), h\,(1+n_2)] \to 0$ leaves $-\frac{1}{hM}$ term uncancelled, nor does it send this term to zero, so simply letting $\psi[h\,(1+n_1), h\,(1+n_2)] \to 0$

results in a broken symmetry

*)

Note that in the non slowly varying case , these terms combine as

$$-\frac{1}{hM}\psi[h\,n_1, h\,n_2] + + \left(\frac{1}{2\mu}+\frac{1}{h\,M}\right)\psi[h\,n_1, h\,(1+n_2)] +$$
$$\left(\frac{1}{2\mu}+\frac{1}{h\,M}\right)\psi[h\,(1+n_1), h\,n_2] - \frac{1}{h\,M}\psi[h\,(1+n_1), h\,(1+n_2)]$$
$$= -\frac{1}{hM}(\psi[h\,(1+n_1), h\,(1+n_2)] + \psi[h\,n_1, h\,n_2]) +$$
$$\left(\frac{1}{2\mu}+\frac{1}{h\,M}\right)\psi[h\,n_1, h\,(1+n_2)] + \left(\frac{1}{2\mu}+\frac{1}{h\,M}\right)\psi[h\,(1+n_1), h\,n_2] ,$$

So the full expression actually has a $\frac{1}{hM}$ dependence,

so it has some symmetry breaking in this regard. With that in mind it ***might actually be more proper to do the Appx*** $\boldsymbol{\psi[h\,(1+n_1), h\,(1+n_2)] \to 0}$ ***in some instances, so as to reproduce this symmetry breaking. Might not reproduce it to scale, but can capture the fundamentals of what ' s happening***

This is an important point,
as it lends some motivation to do this. Futhermore,
this symmetry breaking might be
associated with some physical effect. In that case,
the physical effect cannot be fully explained in the $M \to \infty$ Appx.

$(n_1 - L)\,(n_1 - 2\,L)$ // Expand

$2\,L^2 - 3\,L\,n_1 + n_1^2$

For antisymmetric Appx, we have that,

Then the normalization condition becomes

$$\sum_{n_1,n_2} |\psi(n_1, n_2)|^2 = C < \infty,\ \text{for some finite constant C}$$

In order for the wavefn to describe an actual system
(ie one that lends itself to a probablistic interpretation)