

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

**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}] \*)**

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

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

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

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

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

**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]**

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

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

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

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

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

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

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

$$\begin{aligned}
& \frac{-1}{2\mu} \left( \text{Laplacian}[\psi[x1, y1, z1, x2, y2, z2, t], \{x1, y1, z1, x2, y2, z2\}] \right) - \\
& \left( z (e^2) \left( \frac{1}{\sqrt{x1^2 + y1^2 + z1^2}} + \frac{1}{\sqrt{x2^2 + y2^2 + z2^2}} \right) \psi[x1, y1, z1, x2, y2, z2, t] \right) - \\
& \left( \frac{1}{M} (\text{grad12}) \right) + \frac{(e^2)}{\sqrt{(x1 - x2)^2 + (y1 - y2)^2 + (z1 - z2)^2}} \psi[x1, y1, z1, x2, y2, z2, t] \\
& \frac{e^2 \psi[x1, y1, z1, x2, y2, z2, t]}{\sqrt{(x1 - x2)^2 + (y1 - y2)^2 + (z1 - z2)^2}} - \\
& e^2 z \left( \frac{1}{\sqrt{x1^2 + y1^2 + z1^2}} + \frac{1}{\sqrt{x2^2 + y2^2 + z2^2}} \right) \psi[x1, y1, z1, x2, y2, z2, t] - \\
& \frac{1}{M} \left( \psi^{(\theta, \theta, 1, \theta, \theta, 1, \theta)}[x1, y1, z1, x2, y2, z2, t] + \right. \\
& \quad \psi^{(\theta, 1, \theta, \theta, 1, \theta, \theta)}[x1, y1, z1, x2, y2, z2, t] + \psi^{(1, \theta, \theta, 1, \theta, \theta, \theta)}[x1, y1, z1, x2, y2, z2, t] \left. \right) - \\
& \frac{1}{2\mu} \left( \psi^{(\theta, \theta, \theta, \theta, \theta, 2, \theta)}[x1, y1, z1, x2, y2, z2, t] + \psi^{(\theta, \theta, \theta, \theta, 2, \theta, \theta)}[x1, y1, z1, x2, y2, z2, t] + \right. \\
& \quad \psi^{(\theta, \theta, \theta, 2, \theta, \theta, \theta)}[x1, y1, z1, x2, y2, z2, t] + \psi^{(\theta, \theta, 2, \theta, \theta, \theta, \theta)}[x1, y1, z1, x2, y2, z2, t] + \\
& \quad \psi^{(\theta, 2, \theta, \theta, \theta, \theta, \theta)}[x1, y1, z1, x2, y2, z2, t] + \psi^{(2, \theta, \theta, \theta, \theta, \theta, \theta)}[x1, y1, z1, x2, y2, z2, t] \left. \right) \\
& D[\psi[x1, x2], x1, x2] \rightarrow \\
& \frac{\psi[x1 + h1, x2 + h2] - \psi[x1 + h1, x2] - \psi[x1, x2 + h2] + \psi[x1, x2]}{(h1 h2)}
\end{aligned}$$

$$\begin{aligned}
& \frac{-1}{2\mu} \left( \frac{(\psi[x1 + 2 h1, x2] - \psi[x1 + h1, x2] + \psi[x1, x2])}{h1} + \right. \\
& \quad \left. \frac{(\psi[x1, x2 + 2 h2] - \psi[x1, x2 + h2] + \psi[x1, x2])}{h2} \right) - \left( z (e^2) \left( \frac{1}{x1} + \frac{1}{x2} \right) \right) (\psi[x1, x2]) - \\
& \frac{1}{M} \left( \frac{\psi[x1 + h1, x2 + h2] - \psi[x1 + h1, x2] - \psi[x1, x2 + h2] + \psi[x1, x2]}{(h1 h2)} \right) + \\
& \frac{(e^2)}{\text{Abs}[x2 - x1]} \psi[x1, x2]
\end{aligned}$$

let h1 = h2 = h, x1 = n1 h, x2 = n2 h

$$\begin{aligned}
& \frac{-1}{2\mu} \left( \frac{(\psi[x1 + 2h1, x2] - \psi[x1 + h1, x2] + \psi[x1, x2])}{h1} + \right. \\
& \quad \left. \frac{(\psi[x1, x2 + 2h2] - \psi[x1, x2 + h2] + \psi[x1, x2])}{h2} \right) - \left( z (e^2) \left( \frac{1}{x1} + \frac{1}{x2} \right) \right) (\psi[x1, x2]) - \\
& \quad \frac{1}{M} \left( \frac{1}{(h1 h2)} (\psi[x1 + h1, x2 + h2] - \psi[x1 + h1, x2] - \psi[x1, x2 + h2] + \psi[x1, x2]) \right) + \\
& \quad \frac{(e^2)}{\text{Abs}[(x2 - x1)]} \psi[x1, x2] /. h1 \rightarrow h /. h2 \rightarrow h /. x1 \rightarrow n1 h /. x2 \rightarrow n2 h // Simplify
\end{aligned}$$

$$\begin{aligned}
& \left( \frac{e^2}{\text{Abs}[h(-n1 + n2)]} - \frac{\frac{1}{M} + \frac{h}{\mu} + \frac{e^2 h z}{n1} + \frac{e^2 h z}{n2}}{h^2} \right) \psi[h n1, h n2] + \frac{1}{2 h^2 M \mu} \\
& (-h M \psi[h n1, h(2 + n2)] + (h M + 2 \mu) \psi[h n1, h + h n2] - h M \psi[h(2 + n1), h n2] + \\
& h M \psi[h + h n1, h n2] + 2 \mu \psi[h + h n1, h n2] - 2 \mu \psi[h + h n1, h + h n2])
\end{aligned}$$

$$\begin{aligned}
& \left( \frac{e^2}{\text{Abs}[h(-n1 + n2)]} - \frac{\frac{1}{M} + \frac{h}{\mu} + \frac{e^2 h z}{n1} + \frac{e^2 h z}{n2}}{h^2} \right) \psi[h n1, h n2] + \frac{1}{2 h^2 M \mu} \\
& (-h M \psi[h n1, h(2 + n2)] + (h M + 2 \mu) \psi[h n1, h + h n2] - h M \psi[h(2 + n1), h n2] + \\
& h M \psi[h + h n1, h n2] + 2 \mu \psi[h + h n1, h n2] - 2 \mu \psi[h + h n1, h + h n2]) /. e \rightarrow 1
\end{aligned}$$

$$\begin{aligned}
& \left( \frac{1}{\text{Abs}[h(-n1 + n2)]} - \frac{\frac{1}{M} + \frac{h}{\mu} + \frac{h z}{n1} + \frac{h z}{n2}}{h^2} \right) \psi[h n1, h n2] + \frac{1}{2 h^2 M \mu} \\
& (-h M \psi[h n1, h(2 + n2)] + (h M + 2 \mu) \psi[h n1, h + h n2] - h M \psi[h(2 + n1), h n2] + \\
& h M \psi[h + h n1, h n2] + 2 \mu \psi[h + h n1, h n2] - 2 \mu \psi[h + h n1, h + h n2])
\end{aligned}$$

$$\begin{aligned}
H \psi &= \left( \frac{1}{\text{Abs}[h(-n1 + n2)]} - \frac{\frac{1}{M} + \frac{h}{\mu} + \frac{h z}{n1} + \frac{h z}{n2}}{h^2} \right) \psi[h n1, h n2] + \frac{1}{2 h^2 M \mu} \\
& (-h M \psi[h n1, h(2 + n2)] + (h M + 2 \mu) \psi[h n1, h + h n2] - h M \psi[h(2 + n1), h n2] + \\
& h M \psi[h + h n1, h n2] + 2 \mu \psi[h + h n1, h n2] - 2 \mu \psi[h + h n1, h + h n2])
\end{aligned}$$

$$= \frac{1}{h} \left( \frac{1}{\text{Abs}[(-n1 + n2)]} - \left( \frac{1}{h M} + \frac{1}{\mu} + \frac{z}{n1} + \frac{z}{n2} \right) \right) \psi[h n1, h n2] +$$

$$\begin{aligned}
& \left( -\frac{1}{2 h \mu} \right) (\psi[h n1, h(2 + n2)] + \psi[h(2 + n1), h n2]) + \\
& \left( \frac{1}{2 h \mu} + \frac{1}{h^2 M} \right) \psi[h n1, h(1 + n2)] + \\
& \left( \frac{1}{2 h \mu} + \frac{1}{h^2 M} \right) \psi[h(1 + n1), h n2] - \frac{1}{h^2 M} \psi[h(1 + n1), h(1 + n2)]
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{h} \left( \left( \frac{1}{\text{Abs}[-n_1 + n_2]} - \left( \frac{1}{hM} + \frac{1}{\mu} + \frac{Z}{n_1} + \frac{Z}{n_2} \right) \right) \psi[h n_1, h n_2] + \right. \\
&\quad \left( -\frac{1}{2\mu} \right) (\psi[h n_1, h(2+n_2)] + \psi[h(2+n_1), h n_2]) + \left( \frac{1}{2\mu} + \frac{1}{hM} \right) \psi[h n_1, h(1+n_2)] + \\
&\quad \left. \left( \frac{1}{2\mu} + \frac{1}{hM} \right) \psi[h(1+n_1), h n_2] - \frac{1}{hM} \psi[h(1+n_1), h(1+n_2)] \right)
\end{aligned}$$

(In the  $M \rightarrow \infty$  Appx,  $\mu \rightarrow m$ , and we can see that the

$\psi[h(1+n_1), h(1+n_2)]$  is the only term entirely removed, i.e.  $M \rightarrow$

$\infty$  appx removes symmetric single-site perturbation 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  $M \rightarrow \infty$  Appx

Then, in the Appx where  $\psi$  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 perturbations, we have that

$$\begin{aligned}
H \psi &\approx \left( \left( \frac{1}{\text{Abs}[-n_1 + n_2]} - \left( \frac{1}{hM} + \frac{1}{\mu} + \frac{Z}{n_1} + \frac{Z}{n_2} \right) \right) + \right. \\
&\quad \left( -\frac{1}{2\mu} \right) (2) + \left( \frac{1}{2\mu} + \frac{1}{hM} \right) + \left( \frac{1}{2\mu} + \frac{1}{hM} \right) - \frac{1}{hM} \right) \frac{1}{h} \psi[h n_1, h n_2] \\
&= \left( \left( \frac{1}{\text{Abs}[-n_1 + n_2]} - \left( \frac{1}{hM} + \frac{1}{\mu} + \frac{Z}{n_1} + \frac{Z}{n_2} \right) \right) + \frac{1}{hM} \right) \frac{1}{h} \psi[h n_1, h n_2] \\
&= \left( \frac{1}{\text{Abs}[-n_1 + n_2]} - Z \left( \frac{1}{n_1} + \frac{1}{n_2} \right) - \frac{1}{\mu} \right) \frac{1}{h} \psi[h n_1, h n_2]
\end{aligned}$$

Let  $n_2 = n_1 + L$

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

And for  $n_1 \gg L$  (electrons near each other on the scale of  $L$ ) we have that

(Can also let  $(x_2 - x_1) = hL \sim \xi$  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  $n_1 \sim L$

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

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

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

\*)

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

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

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

$$= -\frac{1}{hM} (\psi[h(1+n_1), h(1+n_2)] + \psi[h n_1, h n_2]) +$$

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

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  $\psi[h(1+n_1), h(1+n_2)] \rightarrow 0$  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. Furthermore,

this symmetry breaking might be

associated with some physical effect. In that case,

the physical effect cannot be fully explained in the  $M \rightarrow \infty$  Appx.

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

$$2L^2 - 3Ln_1 + n_1^2$$

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 probabilistic interpretation)