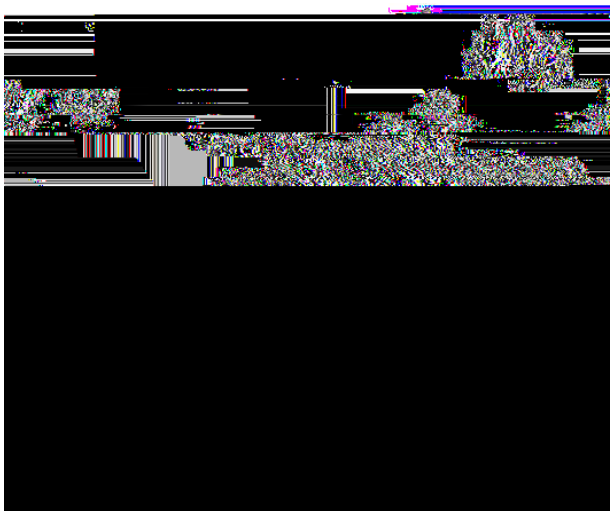
the octopus **manual**

Electronic Structure
Molecular Dynamics
Excited-State Dynamics
Recipes-Generator
March 2002



Male Hapalochlaena lunulata (top),
and female Hapalochlaena lunulata (bottom).

1 Copying

3.2 Time dependent density functional theory

Several reviews of time-dependent density function theory (TDDFT) and its applications have appeared recently, like the works by Gross et al.[2], Casida[3], Dobson et al,[4] , and Burke et al[5].

The Hohenberg-Kohn-Sham theory as described is a ground state theory, and it is hence not meant for the calculation of electronic excitations. However, one can extend the ideas of static DFT. When one asks for the evolution of the system under the influence of a time-

determines the time-dependent density, just as in the Hohenb

4 Installation

browse at `http://nautilus.fis.uc.pt/cgi-bin/cvsweb.cgi/marques/octopus/`**. The**

Section 6.1.7 [Verbose], page 14 and see Section 6.1.8 [Debu

5 The parser

All input opion shud be in a file called “ `inp` **”, in the directory** `octopus` **is run from. Alterntively, if ths fies not fund, standard input is re**

6.1.6 UnitsOutput (string, 'a.u.')

Same as Units**, but only refers to the values in the output files. That is, if** UnitsOutput = "eVA"**, all physical values in the output files will be written in eV and Å.**

6.1.7 Verbose (integer, 30)

Verbosity level of the program. The higher, the more verbose octopus **is.**

- **Oxygen labelled 'O'. Next number is the atomic mass (in atomic mass units), and third field, the atomic number (8, in this case). Afterwar**

–

- f886(o)0.299886(p)0.29urier_space

6.7.1 XFunctional (string, 'LDA')

- XFunctional == 'ZER': **No exchange.**
- XFunctional == 'LDA': **Local density approximation.**
- XFunctional == 'RLDA': **Relativistic LDA.**
- XFunctional == 'PBE': **J.P.Perdew, K.Burke and M.Ernzerhof, PRL**

6.10 Time Dependent

When

the

It may the be demonstrated that the order of the error of the algorithm is the same that the one that we would have by making use of the Exponential Midpoint Rule (EM,

- `10`: **Shape is read from a file.**

  If

6.11.4 GOStep

the

6.13.2 SpecDampMode (string, 'exp')

A damping function may be applied to the input fuction before processing the Fourier

the

8 Undocumented Variables

If you want to use these variables you will have to go to the code to find out what they do. If you do it, please take the time to write a short description and send a patch of the manual to us ;) BTW, some of this variables describe things that may not work, or are under developments, so don't blame us...

- **AnimationSam0099(l)-0.248413(e)-0.2ing**
- **AxisTy00-27.7182(e)-0.231629]TJT*[(o)-659.947(B)-0.342408(o)0.0492351(u)0.32898(n)0.330099(d)0.3**
- **CenterOfInversion**
- **CurrentDFT**
- **KineticCuto**
- **LB94**
  - **_beta**
- **LB94_modified**
- **LB94_threshold**
- **OEP_level**
- **OEP_mixing**
- **OptControlA48413(e)-0.2pha**
- **OptControlEps**
- **OptControlInitLaser**
- **OptControlMaiIter**
- **OutputDuringSCF**
- **OutputELF_FS**
- **OutputWfsSqMod**
- **PeriodicDimensions**
- **RestartFileFormat**
- **ShifKPoints**
- **StaticMagneticField**
- **TDDeltaStrengthMode**
- **TDOutputSpin**
- **V48413(e)-0.2ocalCuto**
- **FromScratch**

```
            functional: non-relativistic
Correlation family    : LDA
            functional: !erdew-Zunger
```

```
C  0.000 -1.396  0.000
C -1.209 -0.698  0.000
C -1.209  0.698  0.000
H  0.000  2.479  0.000
H  2.147  1.240  0.000
H  2.147 -1.240  0.000
H  0.000 -2.479  0.000
H -2.147 -1.240  0.000
H -2.147  1.240  0.000
```

6.4.6 DerivativesSpace **(integer, real_space)** **17**
6.4.7 OrderDerivatives **(integer, 4)** **18**
6.4.8

6.10.6 `TDEvolutionMethod` **(integer, etrs)** **26**
6.10.7 `TDLasers` **(block data)**