

# Quantum Monte-Carlo Studies of Generalized Many-body Systems

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# Goals

- Develop a *general* Quantum Monte-Carlo (QMC) solver for *many-body* systems.
  - Achieved through  $\sim 15000$  lines of object oriented C++.
  - 5000 of which were auto-generated by *SymPy*.
  - Large focus on optimizations.
  - Additional focus on software solutions for handling extreme amounts of data.
  - Focus on readability and being easy to extend.

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  - Additional focus on software solutions for handling extreme amounts of data.
  - Focus on readability and being easy to extend.
- Implement several well-known systems and provide *preliminary* results.
  - Total of five systems simulated for up to 56 particles and 108 degrees of freedom.
  - Efficient simulations on both large scales (abel) and smaller scales (single computational nodes)

# Contents

- 1 The basics of Quantum Monte-Carlo
- 2 Modelled systems
- 3 Results and Discussions

# The basic idea

- Project an arbitrary state down on the exact ground state.
- Model this state by an ensemble of random walkers.
- Simulate the projection using stochastic processes.

# The projection

$$\hat{\mathbf{P}}(\tau) = \exp(-(\hat{\mathbf{H}} - E_0)\tau)$$

$$\hat{\mathbf{P}}(\tau) |\Psi_T\rangle = C_0 |\Psi_0\rangle + \sum_{k=1} \mathcal{C}_k \exp(-\Delta E_k \tau) |\Psi_k\rangle$$

where  $\Delta E_k > 0$  and  $C_k = \langle \Psi_k | \Psi_T \rangle$ .

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where  $\Delta E_k > 0$  and  $C_k = \langle \Psi_k | \Psi_T \rangle$ .

In other words

$$\lim_{\tau \rightarrow \infty} \langle \mathbf{r} | \hat{\mathbf{P}}(\tau) | \Psi_T \rangle = \langle \Psi_0 | \Psi_T \rangle \Psi_0(\mathbf{r}).$$

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Using that

$$\hat{\mathbf{P}}(\tau + \delta\tau) = \exp(-(\hat{\mathbf{H}} - E_0)\delta\tau)\hat{\mathbf{P}}(\tau),$$

yields

$$\begin{aligned}\Phi(\mathbf{r}, \tau + \delta\tau) &\equiv \langle \mathbf{r} | \hat{\mathbf{P}}(\tau + \delta\tau) | \Psi_T \rangle \\ &= \int_{\mathbf{r}'} \langle \mathbf{r} | \exp(-(\hat{\mathbf{H}} - E_0)\delta\tau) | \mathbf{r}' \rangle \Phi(\mathbf{r}', \tau) d\mathbf{r}',\end{aligned}$$

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$$\langle \mathbf{r} | \exp(-(\hat{\mathbf{H}} - E_0)\delta\tau) | \mathbf{r}' \rangle \equiv G(\mathbf{r}', \mathbf{r}; \delta\tau).$$

# The stochastic process

In order to relate the Green's function to well known Markov processes, the exponential is split

$$\begin{aligned}\exp(-(\hat{\mathbf{H}} - E_0)\delta\tau) &= \exp\left(\frac{1}{2}\nabla^2\delta\tau - (\hat{\mathbf{V}} - E_0)\delta\tau\right) \\ &= \exp\left(\frac{1}{2}\nabla^2\delta\tau\right) \exp(-(\hat{\mathbf{V}} - E_0)\delta\tau) \\ &\quad + \mathcal{O}(\delta\tau^2),\end{aligned}$$

which reads *diffusion* and *weighting*.

**Problem:** Requires a priori knowledge of the exact ground state energy  $E_0$ .

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**Solution:** Introduce a *trial energy*  $E_T(\tau)$  instead of  $E_0$  in the Green's function.

**Problem:** The Green's function has singular points in the Coulomb interaction.

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**Solution:** By evolving  $f(\mathbf{r}, \tau) = \Phi(\mathbf{r}, \tau)\Psi_T(\mathbf{r})$  instead of  $\Phi(\mathbf{r}, \tau)$  alone, the singularities are *implicitly* taken care of.

Originally  $\Phi(\mathbf{r}, \tau) = \langle \mathbf{r} | \hat{\mathbf{P}}(\tau) | \Psi_T \rangle$  solves:

$$\frac{\partial \Phi(\mathbf{r}, \tau)}{\partial \tau} = \left[ \frac{1}{2} \nabla^2 - (\hat{\mathbf{V}} - E_T) \right] \Phi(\mathbf{r}, \tau).$$

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*Importance sampled:*

$$\frac{\partial f(\mathbf{r}, \tau)}{\partial \tau} = \left[ \frac{1}{2} \nabla \cdot (\nabla - \mathbf{F}(\mathbf{r})) - (E_L(\mathbf{r}) - E_T) \right] f(\mathbf{r}, \tau),$$

where

$$\mathbf{F}(\mathbf{r}) = 2\Psi_T(\mathbf{r})^{-1} \nabla \Psi_T(\mathbf{r})$$

is the *quantum force* and

$$E_L(\mathbf{r}) = \Psi_T(\mathbf{r})^{-1} \hat{\mathbf{H}} \Psi_T(\mathbf{r})$$

is the *local energy*.

The Green's functions have closed form solutions on the form

$$G_{\text{Diff}}(\mathbf{r}', \mathbf{r}; \delta\tau) \propto \exp\left(-|\mathbf{r} - \mathbf{r}' - D\delta\tau\mathbf{F}(\mathbf{r})|^2 / 4D\delta\tau\right),$$

$$G_W(\mathbf{r}', \mathbf{r}; \delta\tau) \propto \exp\left(-\left(\frac{1}{2} [E_L(\mathbf{r}) + E_L(\mathbf{r}')] - E_T\right)\delta\tau\right),$$

where W denotes *weighting*.

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where W denotes *weighting*.

$\Psi_T(\mathbf{r})$  is tailored to cancel singularities in  $E_L(\mathbf{r})$ .

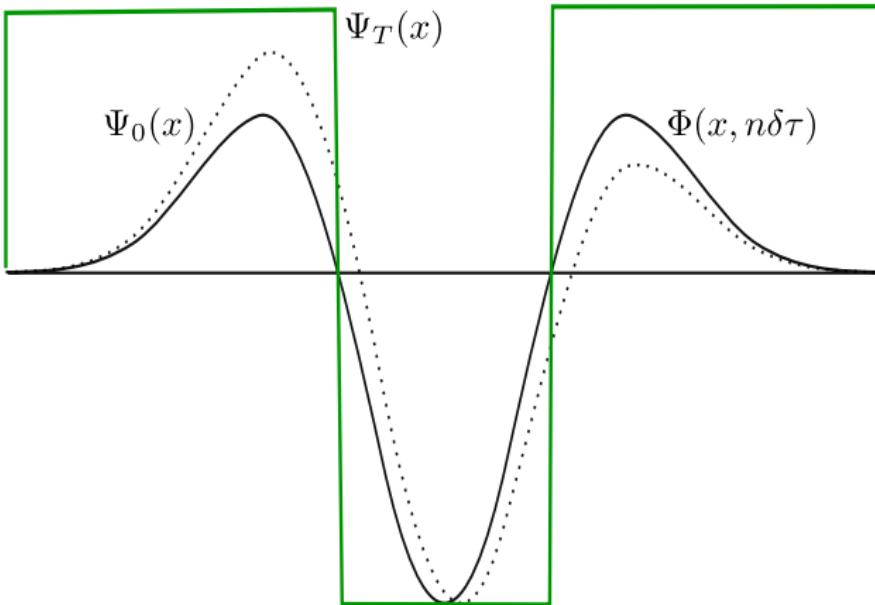
# The Markov process

**Problem:** The distribution  $f(\mathbf{r}, \tau) = \Phi(\mathbf{r}, \tau)\Psi_T(\mathbf{r})$  is not exclusively positive unless the nodes (zeros) of  $\Psi_T(\mathbf{r})$  matches those of  $\Phi(\mathbf{r}, \tau)$ .

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**Solution:** Fixing the nodes of  $f(\mathbf{r}, \tau)$  to match those of  $\Psi_T(\mathbf{r})$  (the *fixed node approximation*).



**Figure:** The fixed node approximation illustrated. The nodes of  $\Phi(x, n\delta\tau)$  is fixed to match those of  $\Psi_T(x)$ .

# Branching

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**Solution:** The walker branch floor( $G_B$ ) times with a chance of one additional copy.

If zero branches, the walker is removed.

# Branching

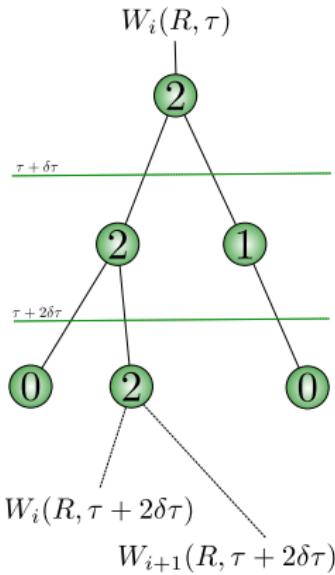


Figure: Branching illustrated. The integer values represent  $\bar{G}_B$ .

# Diffusion

According to the introduced diffusion process, the new position  $\mathbf{r}_{i+1}$  is calculated from the old one,  $\mathbf{r}_i$ , as follows

$$\mathbf{r}_{i+1} = \mathbf{r}_i + D\delta\tau\mathbf{F}(\mathbf{r}_i) + \xi,$$

where  $\xi$  is a vector of normal distributed random numbers with variance  $\sqrt{2D\delta\tau}$ .

# Diffusion

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**Solution:** The *Metropolis algorithm* will correct this bias:

$$A(i \rightarrow j) = \min\{R_G(i \rightarrow j)R_\psi(i \rightarrow j)^2, 1\},$$

where  $i \rightarrow j$  denotes a transition from state  $i$  to state  $j$ ,  $A$  is the probability of accepting the transition,

$$R_G(i \rightarrow j) = G_{\text{Diff}}(\mathbf{r}_j, \mathbf{r}_i; \delta\tau)/G_{\text{Diff}}(\mathbf{r}_i, \mathbf{r}_j; \delta\tau),$$

and

$$R_\psi(i \rightarrow j) = |\Psi_T(\mathbf{r}_j)/\Psi_T(\mathbf{r}_i)|.$$

# Recap

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# Recap

- The distribution at any stage is given as the histogram of the walkers' configurations.
- The projection process involves diffusing the walkers and calculating weights.
- Efficient sampling by using the quantum force.
- Unbiased sampling by using the Metropolis algorithm.
- Transition from  $|\Psi_T|^2 \rightarrow f(\mathbf{r}, \tau)$  by including the weights.

# Variational Monte-Carlo

Neglecting the branching results in a method known as *Variational Monte-Carlo* (VMC).

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Neglecting the branching results in a method known as *Variational Monte-Carlo* (VMC).

Corresponds to calculating  $\langle \Psi_T | \hat{\mathbf{H}} | \Psi_T \rangle$  using a standard Monte-Carlo approach

$$\langle \Psi_T | \hat{\mathbf{H}} | \Psi_T \rangle = \int_{\mathbf{r}} |\Psi_T(\mathbf{r})|^2 E_L(\mathbf{r}) d\mathbf{r} \simeq \frac{1}{N} \sum_{i=1}^N \frac{1}{\Psi_T(\mathbf{r}_i)} \hat{\mathbf{H}} \Psi_T(\mathbf{r}_i)$$

# Variational Monte-Carlo

Variational Monte-Carlo will always result in an energy which is greater or equal to the exact ground state energy

$$\begin{aligned}\langle \Psi_T | \hat{\mathbf{H}} | \Psi_T \rangle &= \sum_{ij} C_i^* C_j \underbrace{\langle \Psi_i | \hat{\mathbf{H}} | \Psi_j \rangle}_{E_i \delta_{ij}} \\ &= \sum_i |C_i|^2 E_i \\ &= \sum_i |C_i|^2 (E_0 + \Delta E_i) \\ &= E_0 \underbrace{\sum_i |C_i|^2}_1 + \underbrace{\sum_i |C_i|^2 \Delta E_i}_{\geq 0} \\ &\geq E_0.\end{aligned}$$

# Limitations: VMC

VMC is extremely robust, however, extremely dependent on a good ansatz for  $\Psi_T(\mathbf{r})$ .

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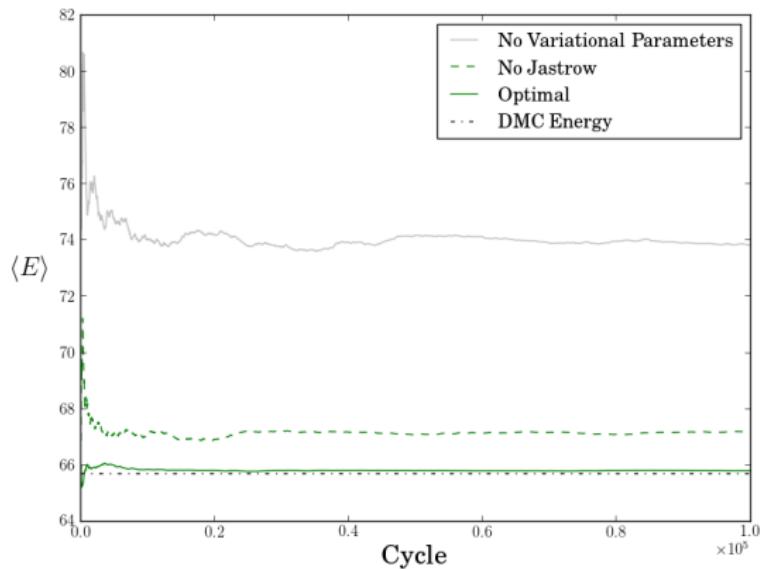


Figure: Comparison of different trial wave functions for a two-dimensional 12-particle quantum dot with unit frequency.

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Including both diffusion and branching results in a method known as *Diffusion Monte-Carlo* (DMC).

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The DMC energy corresponds to the following integral

$$E_{\text{DMC}} = \frac{\int_{\mathbf{r}} f(\mathbf{r}, \tau) \frac{1}{\Psi_T(\mathbf{r})} \hat{\mathbf{H}} \Psi_T(\mathbf{r}) d\mathbf{r}}{\int_{\mathbf{r}} f(\mathbf{r}, \tau) d\mathbf{r}} = \frac{\langle \Phi(\tau) | \hat{\mathbf{H}} | \Psi_T \rangle}{\langle \Phi(\tau) | \Psi_T \rangle},$$

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which upon convergence of the projection results in  
 $\hat{\mathbf{H}} |\Phi(\tau)\rangle = E_0 |\Phi(\tau)\rangle$ . The energy becomes

$$E_{\text{DMC}} = \frac{\langle \Phi(\tau) | E_0 | \Psi_T \rangle}{\langle \Phi(\tau) | \Psi_T \rangle} = E_0.$$

# Limitations: DMC

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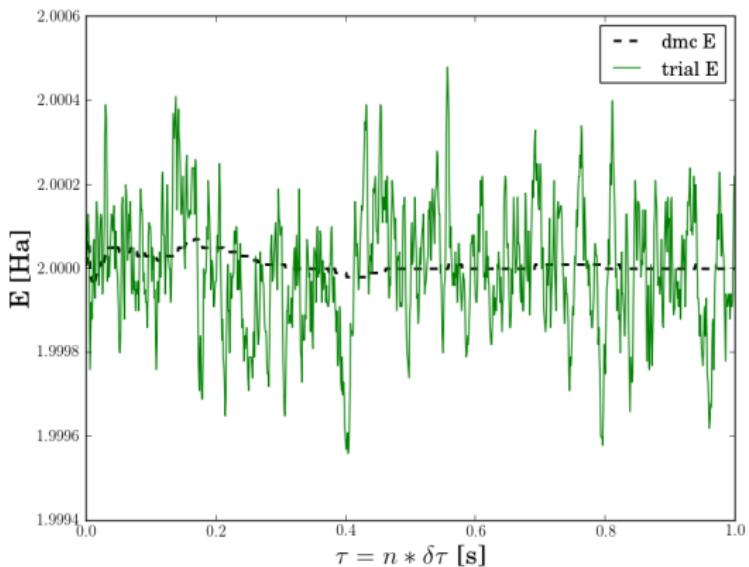
Can be countered by choosing a lower time step.

$$G_W \sim \exp(\sigma(E)\delta\tau)$$

Low  $\delta\tau$  means slower convergence. Unable to span the whole space.

# Limitations: DMC

Diffusion Monte-Carlo is not as dependent on the trial wave function as VMC.



**Figure:** DMC calculation without the exact wave function. The exact result is  $E_0 = 2$ . The VMC energy is  $2.0042(3)$ , whereas the DMC energy is  $2.00000(2)$ .

# The modelled systems

- Quantum dots: Confined electrons
  - Two dimensions
  - Three dimensions
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- Atomic systems
  - Atoms
  - Homonuclear Diatomic Molecules

# Quantum dots

Model the confinement using a harmonic oscillator potential

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The harmonic oscillator eigenfunctions are

$$\phi_{n_x, n_y, n_z}(\mathbf{r}) = H_{n_x}(\sqrt{\omega}x)H_{n_y}(\sqrt{\omega}y)H_{n_z}(\sqrt{\omega}z)e^{-\frac{1}{2}\omega r^2},$$

which serves as the starting ground for creating an ansatz for  $\Psi_T(\mathbf{r})$ .

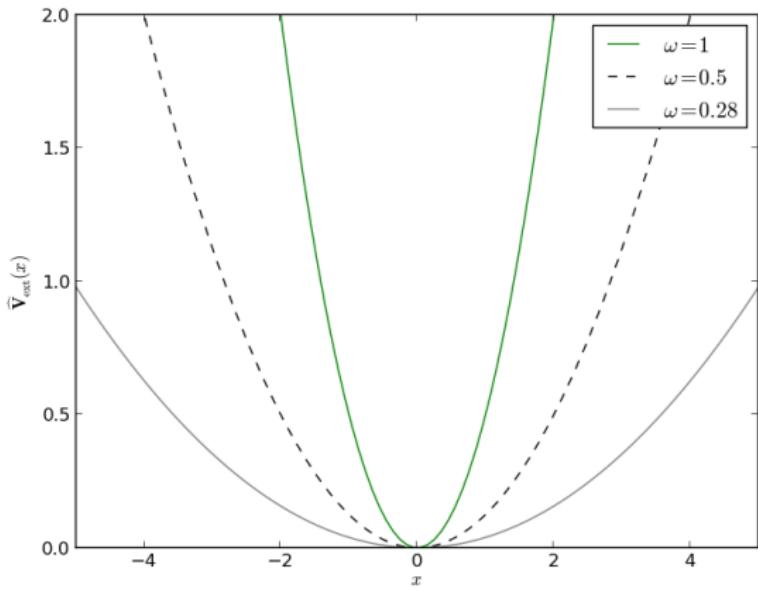


Figure: A one-dimensional version of the single-particle potential of quantum dots.

# Double wells

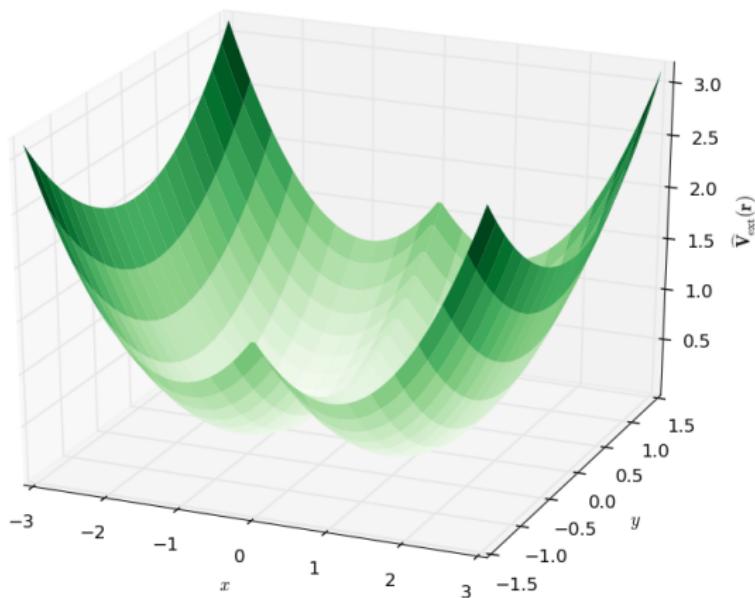


Figure: The external potential for a double-well quantum dot.

# Atomic systems

Atoms are modelled with a Coulomb interaction between the electrons and the nucleus

$$V_{\text{ext}}(\mathbf{r}) = -\frac{Z}{r}.$$

The nucleus is fixed at the origin (the *Born-Oppenheimer Approximation*).

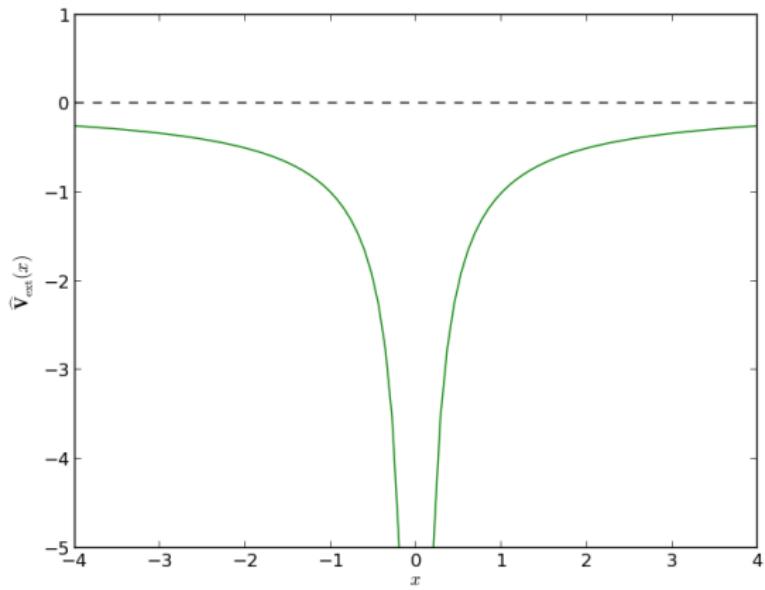


Figure: The one-dimensional version of the single-particle potential of hydrogen.

The eigenfunctions are

$$\phi_{nlm}(r, \theta, \phi; Z) \propto r^l e^{-Zr/n} \left[ L_{n-l-1}^{2l+1} \left( \frac{2r}{n} Z \right) \right] Y_l^m(\theta, \phi).$$

$L_{q-p}^p(x)$ : Associated Laguerre polynomials

$Y_l^m(\theta, \phi)$ : Spherical harmonics.

**Issue:** The spherical harmonics are complex functions.

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**Solution:** Use the *solid harmonics*

$$\begin{aligned} S_l^m(r, \theta, \phi) &\propto r^l [Y_l^m(\theta, \phi) + (-1)^m Y_l^{-m}(\theta, \phi)] \\ &\propto r^l P_l^{|m|}(\cos \theta) \begin{cases} \cos m\phi & m \geq 0 \\ \sin |m|\phi & m < 0 \end{cases}. \end{aligned}$$

The resulting eigenfunctions become

$$\phi_{nlm}(r, \theta, \phi; Z) \propto e^{-Zr/n} \left[ L_{n-l-1}^{2l+1} \left( \frac{2r}{n} Z \right) \right] S_l^m(r, \theta, \phi) \equiv \phi_{nlm}^H(\mathbf{r}).$$

# Molecules

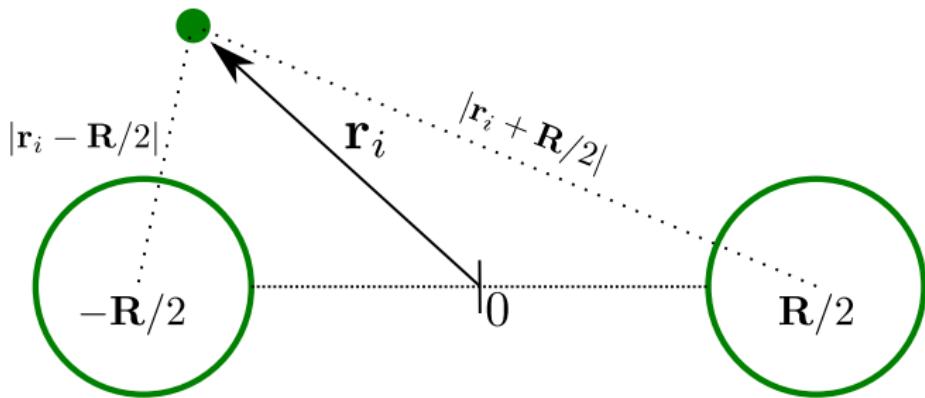


Figure: The model for the diatomic molecule.

The Hamiltonian describing the homonuclear diatomic molecules becomes

$$\hat{\mathbf{H}}_{\text{Mol.}}(\mathbf{r}, \mathbf{R}) = \sum_{i=1}^N \left[ -\frac{1}{2} \nabla_i^2 + \frac{Z}{|\mathbf{r}_i + \mathbf{R}/2|} + \frac{Z}{|\mathbf{r}_i - \mathbf{R}/2|} \right] + \frac{Z^2}{R} + \sum_{i < j} \frac{1}{r_{ij}}$$

A transformation of the single-nucleus hydrogen eigenstates are needed:

$$\begin{aligned}\phi_{nlm}^+(\mathbf{r}_i, \mathbf{R}) &= \phi_{nlm}^H(\mathbf{r}_i + \mathbf{R}/2) + \phi_{nlm}^H(\mathbf{r}_i - \mathbf{R}/2), \\ \phi_{nlm}^-(\mathbf{r}_i, \mathbf{R}) &= \phi_{nlm}^H(\mathbf{r}_i + \mathbf{R}/2) - \phi_{nlm}^H(\mathbf{r}_i - \mathbf{R}/2).\end{aligned}$$

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The same transformation is used to transform the harmonic oscillator eigenfunctions into the double well basis.

$\omega$	E <sub>VMC</sub>	E <sub>DMC</sub>	E <sub>FCI</sub>
0.01	<b>0.07406(5)</b>	<b>0.073839(2)</b>	0.07383505
0.1	<b>0.44130(5)</b>	<b>0.44079(1)</b>	0.44079191
0.28	<b>1.02215(5)</b>	<b>1.02164(1)</b>	1.0216441
0.5	<b>1.66021(5)</b>	<b>1.65977(1)</b>	1.6597723
1.0	<b>3.00030(5)</b>	<b>3.00000(1)</b>	3.0000001

**Figure:** Two-particle results for two-dimensional quantum dots compared with FCI results by Veronica K.B. Olsen.

N	$\omega$	E <sub>VMC</sub>	E <sub>DMC</sub>	E <sub>SRG</sub>	E <sub>CCSD</sub>
42	0.1	107.881(1)	107.6389(2)	-	111.7170 {8}
	0.28	220.161(1)	219.8426(2)	219.8836 {14}	222.1401 {8}
	0.5	331.002(1)	330.6306(2)	330.6485 {14}	331.8901 {8}
	1.0	544.2(8)	542.9428(8)	542.9528 {14}	543.1155 {18}
56	0.1	176.269(2)	175.9553(7)	-	186.1034 {9}
	0.28	358.594(2)	358.145(2)	-	363.2048 {9}
	0.5	538.5(6)	537.353(2)	-	540.3430 {9}
	1	880.2(7)	879.3986(6)	-	879.6386 {17}

**Figure:** Results for two-dimensional quantum dots 42 and 56 particles compared with SRG results by Sarah Reimann and CCSD results by Christoffer Hirth.

N	$\omega$	E <sub>VMC</sub>	E <sub>DMC</sub>	E <sub>0</sub>
2	0.01	0.07939(3)	0.079206(3)	-
	0.1	0.50024(8)	0.499997(3)	0.5
	0.28	1.20173(5)	1.201725(2)	-
	0.5	2.00005(2)	2.000000(2)	2.0
	1.0	3.73032(8)	3.730123(3)	-

**Figure:** Results for three-dimensional quantum dots compared with exact solutions by M. Taut.

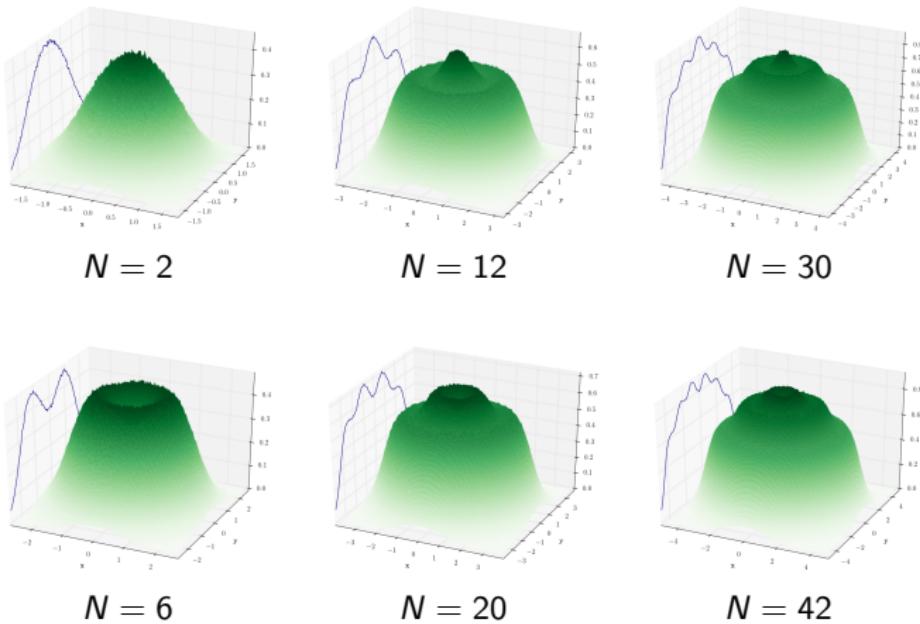


Figure: DMC one-body densities for two-dimensional quantum dots.



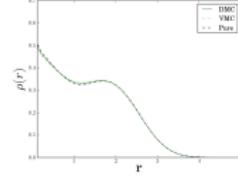
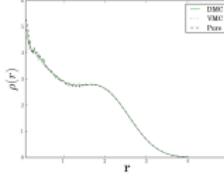
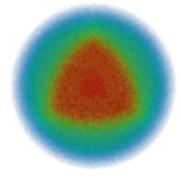
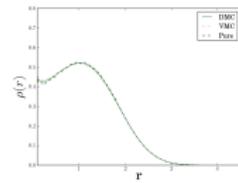
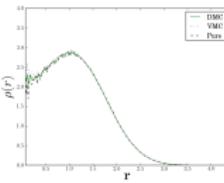
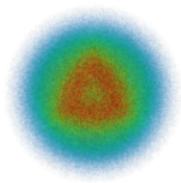
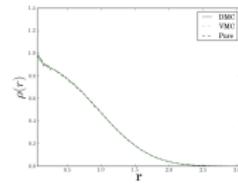
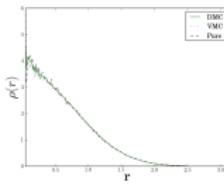
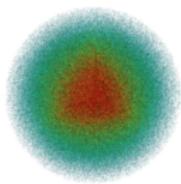


Figure: One-body densities for two- and three-dimensional quantum dots.

# Lowering the frequency

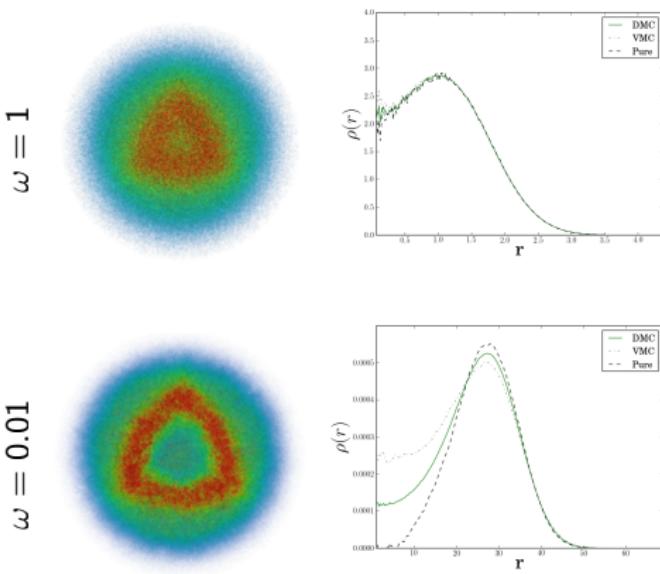
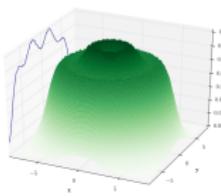
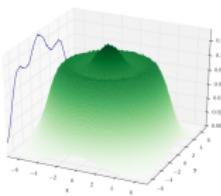
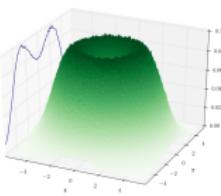
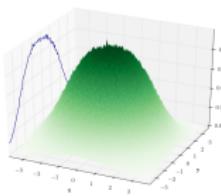
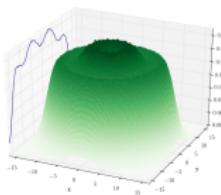
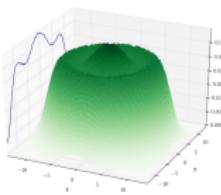
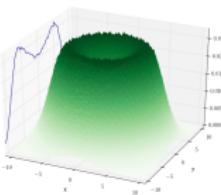
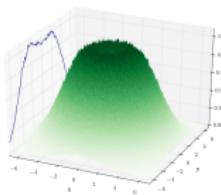


Figure: One-body densities for a 8-particle three-dimensional quantum dot for high and low frequencies.

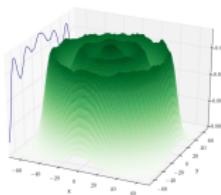
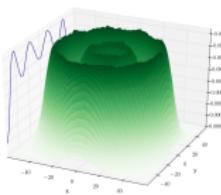
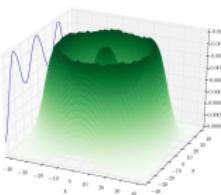
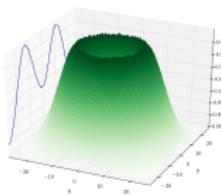
$\omega = 0.28$



$\omega = 0.1$



$\omega = 0.01$



$N = 2$

$N = 6$

$N = 12$

$N = 20$

The electrons become more *localized* and dilute.

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The two- and three-dimensional densities no longer match.

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Transition into a new region?

# Electron crystals for N=6

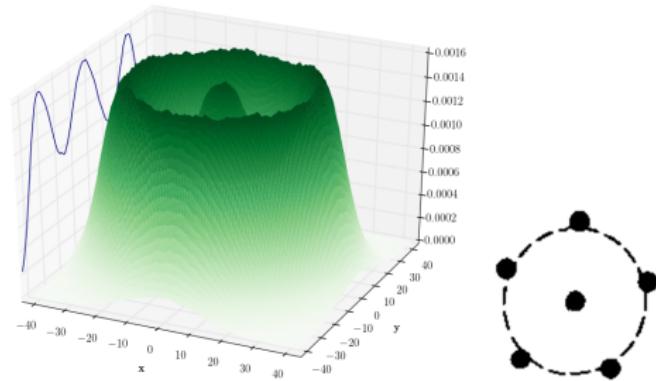


Figure: OBD for a 6-particle two-dimensional quantum dot compared to the classical theoretical configuration taken from F. Bolton, U. Rössler. *Superlattices and microstructures* **13**, 139 (1993).

# Electron crystals for N=6 (frozen)

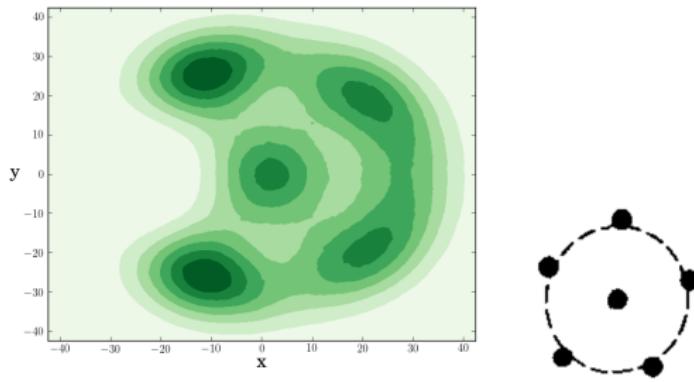


Figure: OBD for a 6-particle two-dimensional quantum dot compared to the classical theoretical configuration taken from F. Bolton, U. Rössler. *Superlattices and microstructures* **13**, 139 (1993).

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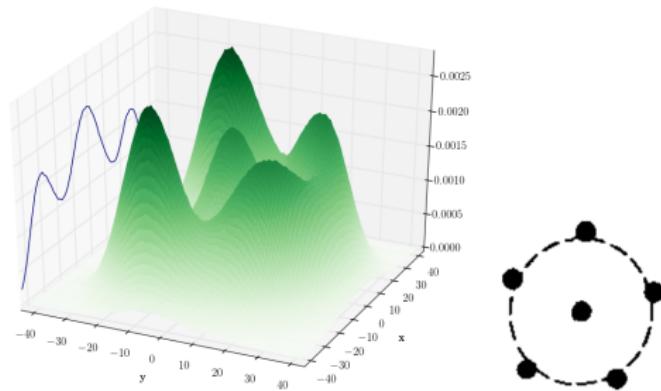


Figure: OBD for a 6-particle two-dimensional quantum dot compared to the classical theoretical configuration taken from F. Bolton, U. Rössler. *Superlattices and microstructures* **13**, 139 (1993).

# Electron crystals for N=12

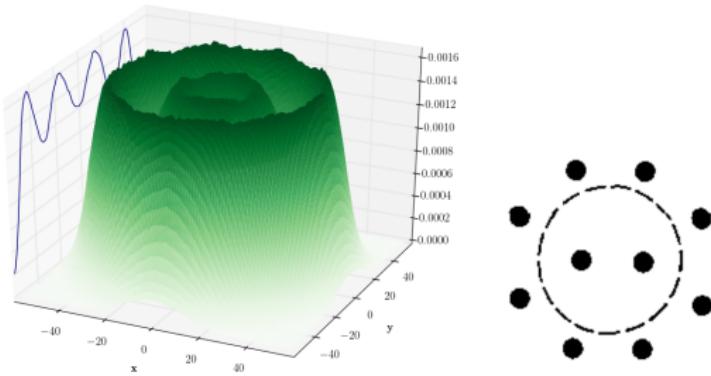


Figure: OBD for a 12-particle two-dimensional quantum dot compared to the classical theoretical configuration taken from F. Bolton, U. Rössler. *Superlattices and microstructures* **13**, 139 (1993).

# Electron crystals for N=12 (frozen)

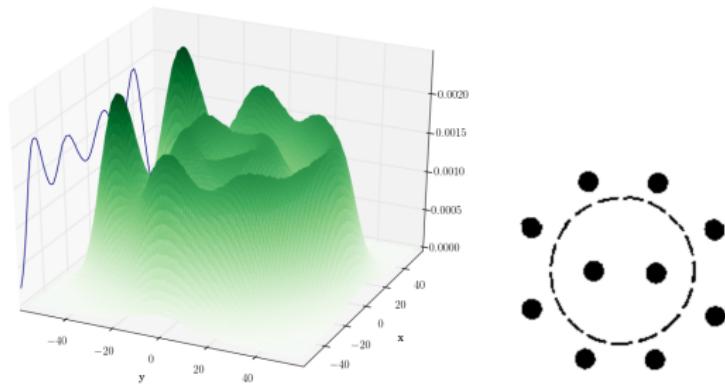


Figure: OBD for a 12-particle two-dimensional quantum dot compared to the classical theoretical configuration taken from F. Bolton, U. Rössler. *Superlattices and microstructures* **13**, 139 (1993).

# Electron crystals N=20

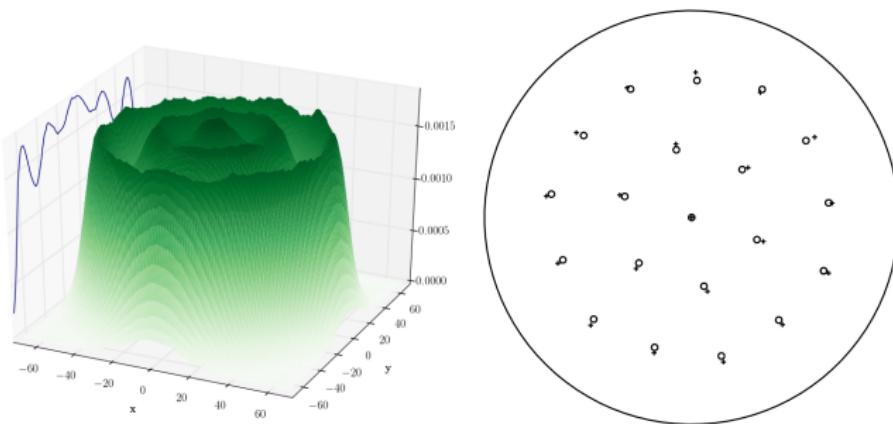


Figure: OBD for a 20-particle two-dimensional quantum dot compared to the classical theoretical configuration taken from P. Galatola et al. *Eur. Phys. J. B* **50**, 549 (2006).

This effect is called *Wigner Crystallization* and is expected for low density electron gases when the **kinetic energy on average becomes far lower than the corresponding total potential energy.**

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The connection between potential and kinetic energy is given by the *virial theorem*

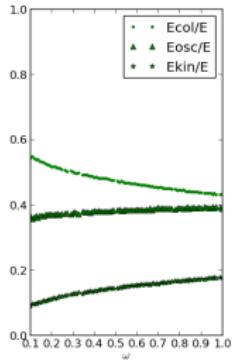
$$V(\mathbf{r}) \propto r^\gamma \quad \longrightarrow \quad \langle \hat{\mathbf{T}} \rangle = \frac{\gamma}{2} \langle \hat{\mathbf{V}} \rangle, \quad (1)$$

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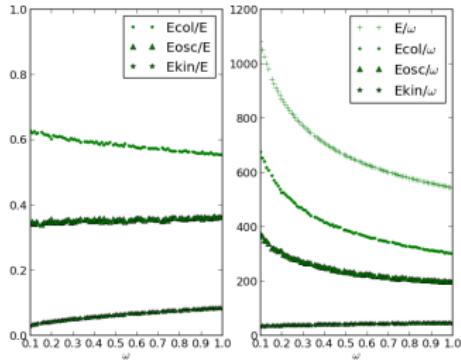
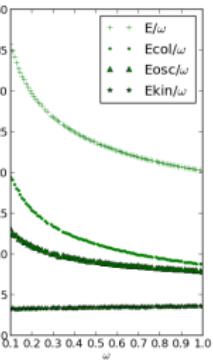
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$$V(r) \propto r^\gamma \quad \longrightarrow \quad \langle \hat{\mathbf{T}} \rangle = \frac{\gamma}{2} \langle \hat{\mathbf{V}} \rangle, \quad (1)$$

Systems with similar proportionality constant follow the same effective potential, that is, they have similar eigenstates.



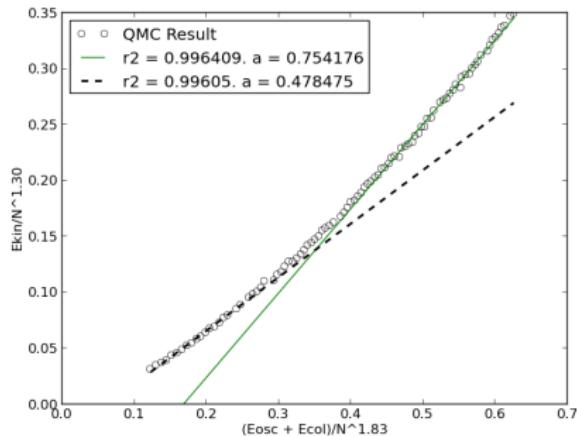
$N = 6$



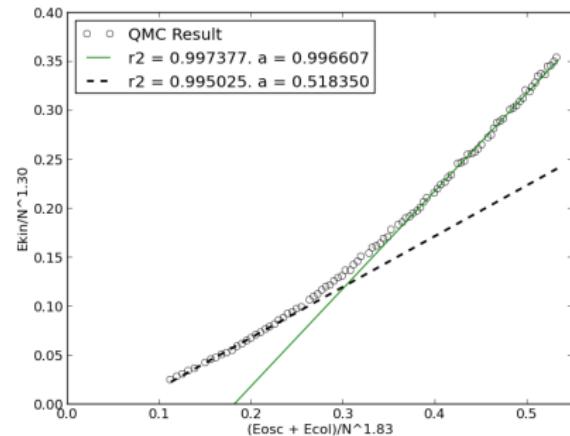
$N = 42$

**Figure:** The relative magnitude of the expectation value of the different energy sources as a function of the frequency  $\omega$  (left) together with the magnitude of the sources' energy contributions scaled with the oscillator frequency (right).

# Transition into a Wigner crystal?



$N = 6$



$N = 42$

**Figure:** The total kinetic energy vs. the total potential energy of two dimensional quantum dots. NB: Collapsed.

# Preliminary double-well density

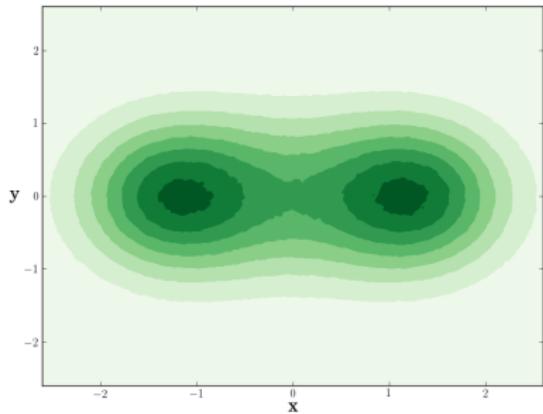


Figure: A countour plot of the trial wave function for a two-particle double-well quantum dot with the wells separated at a distance  $R = 2$ .

# Atoms

Atom (N)	$E_{\text{VMC}}$	$E_{\text{DMC}}$	Expt.
He (2)	-2.8903(2)	-2.9036(2)	-2.9037
Kr (36)	-2700(5)	-2749.9(2)	-2752.054976

Table: Ground state energies for atoms calculated using Variational - and Diffusion Monte-Carlo.

# Densities: The noble gases

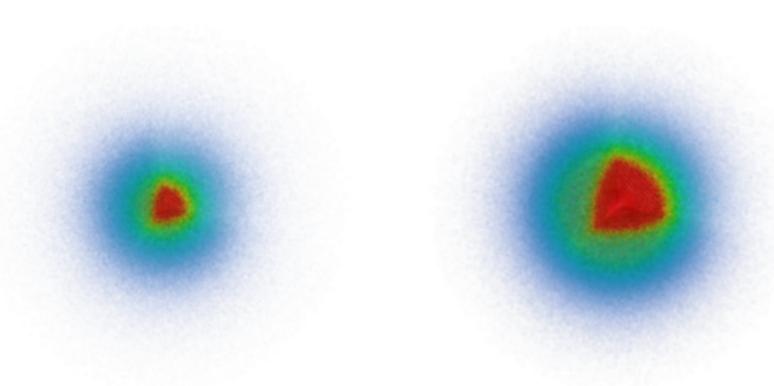
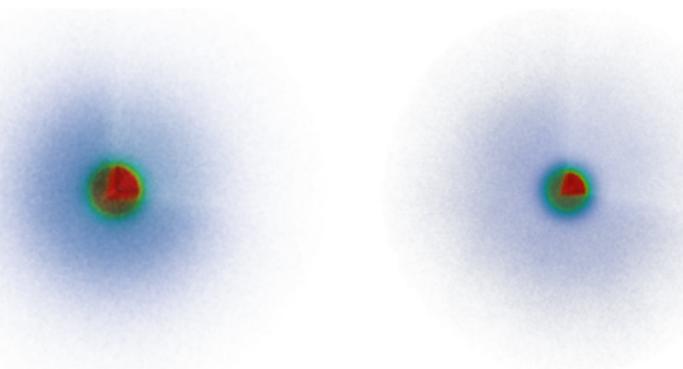


Figure: One-body densities for helium and neon.

# Densities: The alkaline earth metals



**Figure:** Three dimensional one-body density for alkaline earth metals; beryllium and magnesium.

# Molecules

Molecule (N)	$R$	$E_{\text{VMC}}$	$E_{\text{DMC}}$	Expt.
H <sub>2</sub> (2)	1.4	-1.1551(3)	-1.1745(3)	-1.1746
O <sub>2</sub> (16)	2.282	-143.97(2)	-148.53(2)	-150.3268

**Table:** Ground state energies for homonuclear diatomic molecules calculated using VMC and DMC.

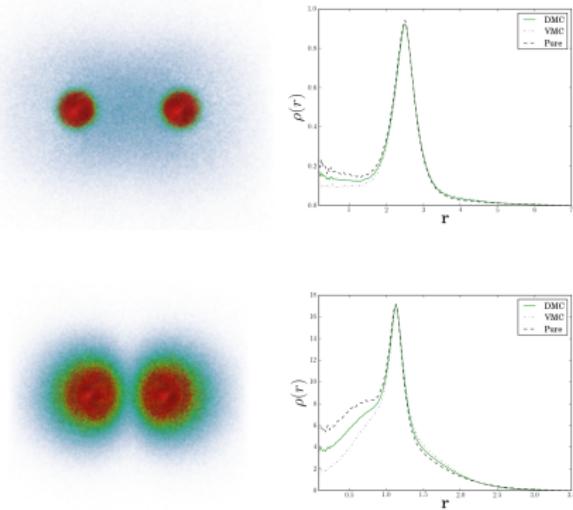


Figure: One-body densities of Li<sub>2</sub> (top) and O<sub>2</sub> (bottom).

# Parameterizing force-field potentials

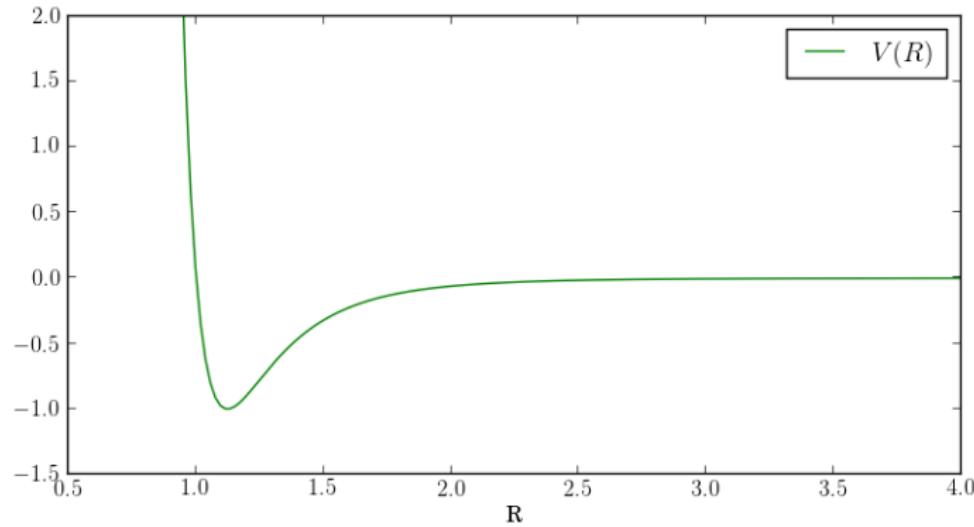
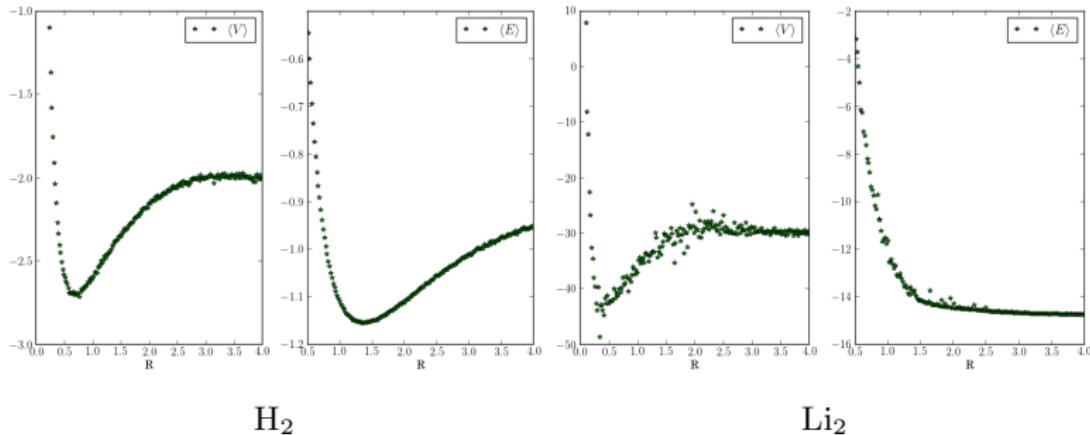


Figure: The Lennard-Jones 12-6 potential.

# Parameterizing force-field potentials



**Figure:** The distance between the atoms  $R$  vs. the potential and total energy calculated using QMC.

# Prospects and future work

- Investigate the similarities between two- and three-dimensional quantum dots in greater detail.
- Perform a detailed QMC analysis of double-well quantum dots.
- Study more complicated molecules.
  - Expand the code to general molecules.
  - Obtain a better atomic trial wave function by using *Hartree-Fock* or Coupled Cluster wave functions.
- Implement a momentum space version of QMC for studying nuclear interactions in great detail.