

Quantum Monte-Carlo Studies of Generalized Many-body Systems

Jørgen Høgberget

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 - 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 Results and Discussions

Unfamiliar with Quantum Mechanics?

Imagine states as vectors and operators as matrices:

$$|\Psi\rangle \rightarrow \begin{pmatrix} a \\ b \end{pmatrix}.$$

$$\langle\Psi| \rightarrow (a^*, b^*).$$

$$\hat{\mathbf{H}} \rightarrow \begin{pmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{pmatrix}.$$

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Ground state: Corresponding eigenvector $|\Psi_0\rangle$.

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

In other words

$$\lim_{\tau \rightarrow \infty} \langle \mathbf{r} | \hat{\mathbf{P}}(\tau) | \Psi_T \rangle = \langle \Psi_0 | \Psi_T \rangle \Psi_0(\mathbf{r}). \quad (1)$$

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Solution: Introduce a *trial energy* $E_T(\tau)$. Will work as long as the trial energy drops below E_1 at a certain stage (and stays there).

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This is achieved by using the following property of the projection operator

$$\begin{aligned}\hat{\mathbf{P}}(\tau + \delta\tau) &= \exp(-(\hat{\mathbf{H}} - E_T(\tau + \delta\tau))(\tau + \delta\tau)) \\ &= \exp(-(\hat{\mathbf{H}} - E_T(\tau + \delta\tau))\delta\tau) \\ &\quad \times \exp(-(\hat{\mathbf{H}} - E_T(\tau + \delta\tau))\tau)\end{aligned}$$

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where the relation is approximate due to E_T not being constant.

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where $\langle \mathbf{r} | \exp(-(\hat{\mathbf{H}} - E_T)\delta\tau) | \mathbf{r}' \rangle \equiv G(\mathbf{r}', \mathbf{r}; \delta\tau)$ is a *Green's function* interpreted as the transition probability between \mathbf{r} and \mathbf{r}' .

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

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

where the kinetic part describes a diffusion process with diffusion constant $D = \frac{1}{2}$, and the potential part describes a weighting (linear in position space). This is referred to as the *short time approximation*.

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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:

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

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Importance sampled:

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

where

$$\mathbf{F}(\mathbf{r}) = 2\psi_T(\mathbf{r})^{-1} \nabla \psi_T(\mathbf{r}) \quad (3)$$

is the *quantum force* and

$$E_L(\mathbf{r}) = \psi_T(\mathbf{r})^{-1} \hat{\mathbf{H}} \psi_T(\mathbf{r}) \quad (4)$$

is the *local energy*.

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

$$G_{\text{Diff}}(\mathbf{r}', \mathbf{r}; \delta\tau) \propto \exp\left(-|\mathbf{r} - \mathbf{r}' - D\delta\tau\mathbf{F}(\mathbf{r})|^2 / 4D\delta\tau\right),$$
$$G_B(\mathbf{r}', \mathbf{r}; \delta\tau) \propto \exp\left(-\left(\frac{1}{2} [E_L(\mathbf{r}) + E_L(\mathbf{r}')] - E_T\right)\delta\tau\right),$$

where B denotes *branching*.

The local energy dependence in the branching Green's function implicitly takes care of the singularities in \hat{V} .

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This is done by introducing the *Jastrow factor* in $\Psi_T(\mathbf{r})$

$$J(\mathbf{r}) = \prod_{i>j}^N \exp \left(a_{ij} \frac{r_{ij}}{1 + \beta r_{ij}} \right), \quad (5)$$

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, N is the number of particles, β is a variational parameter, and a_{ij} is a constant depending on the spin eigenvalues of particles i and j .

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The Jastrow factor is tailored to cancel the singularities in the electron-electron Coulomb interaction as the relative distances decrease.

The Markov process

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Solution: By *fixing* the nodes of $f(\mathbf{r}, \tau)$ to match those of $\Psi_T(\mathbf{r})$, the nodes of $\Phi(\mathbf{r}, \tau)$ will consequently match these as well. This is known as the *fixed node approximation* (FNA).

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Consequence: If the FNA is not redundant, $\Phi(\mathbf{r}, \tau)$ will never converge to the exact ground state.

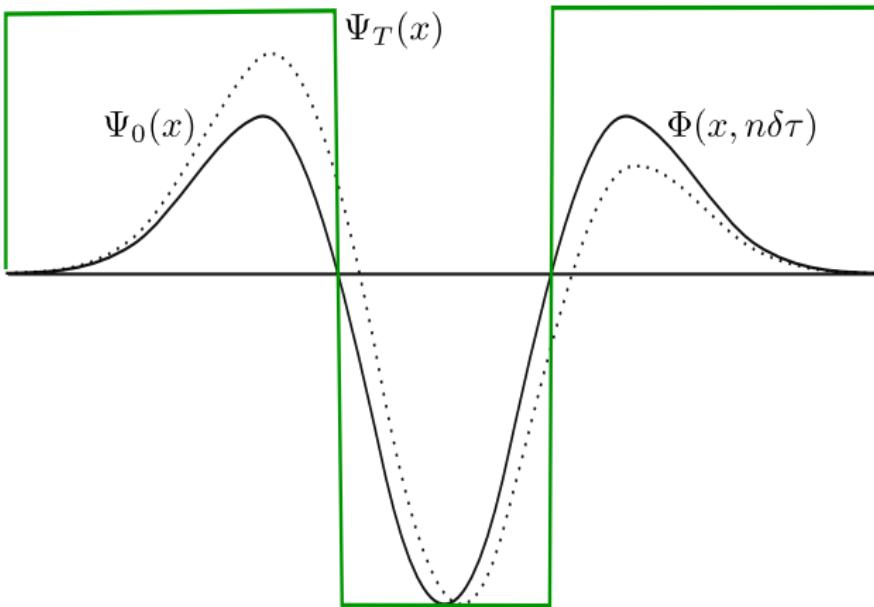


Figure: The fixed node approximation illustrated. The nodes of $\Phi(x, n\delta\tau)$ is fixed to match those of $\Psi_T(x)$.

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Or more compact: Create

$$\bar{G}_B = \text{floor}(G_B + a) \quad (6)$$

copies, where $a \in [0, 1]$ is a uniformly distributed random number.
If the value is zero, the walker dies.

Branching

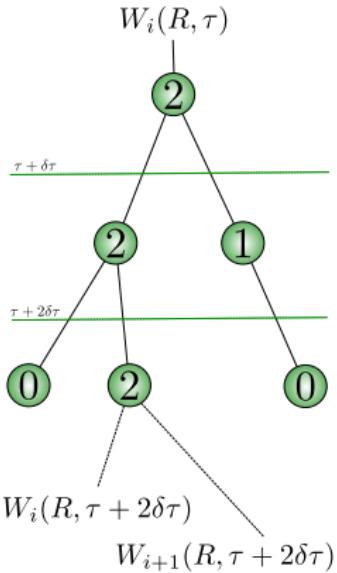


Figure: Branching illustrated. The integer values represent \overline{G}_B .

Diffusion

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Anisotropic diffusion process. The quantum force pushes the walkers into regions of higher probability.

According to the Fokker-Planck formalism, a new position \mathbf{r}_{i+1} is calculated from the old one, \mathbf{r}_i , as follows

$$\mathbf{r}_{i+1} = \mathbf{r}_i + D\delta\tau \mathbf{F}(\mathbf{r}_i) + \xi, \quad (7)$$

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

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

$$A(i \rightarrow j) = \min\{R_G(i \rightarrow j)R_\psi(i \rightarrow j)^2, 1\}, \quad (8)$$

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 projection process is approximated by the diffusion of an ensemble of walkers with distributed weights.
- Diffusion by the Fokker-Planck equation ensures efficient sampling by the use of the quantum force.
- The Metropolis algorithm corrects the bias introduced by a finite step length. Ensures that the walkers follow $|\Psi_T(\mathbf{r})|^2$.
- After each diffusion step, the walker is either killed or cloned based on the value of the branching Green's function. This ensures that the distribution of walkers follows $f(\mathbf{r}, \tau)$ and not $|\Psi_T(\mathbf{r})|^2$.

Variational Monte-Carlo

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

$$\langle \Psi_T | \hat{\mathbf{H}} | \Psi_T \rangle = \int_{\mathbf{r}} |\Psi_T(\mathbf{r})|^2 E_L(\mathbf{r}) d\mathbf{r} \simeq \frac{1}{N} \sum_{i=1}^N \frac{1}{\Psi_T(\mathbf{r}_i)} \hat{\mathbf{H}} \Psi_T(\mathbf{r}_i) \quad (9)$$

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Notice that using any other distribution than $|\Psi_T(\mathbf{r})|^2$ to sample the points \mathbf{r}_i results in undefined samples of the local energy.

Variational Monte-Carlo

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

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

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Introducing the variational parameter α into the spatial wave function yields

$$\Psi_T(\mathbf{r}; \alpha, \beta) = |\mathbf{S}(\mathbf{r}; \alpha)^\uparrow| |\mathbf{S}(\mathbf{r}; \alpha)^\downarrow| J(\mathbf{r}; \beta) \quad (10)$$

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$$E_{\text{DMC}} = \frac{\int_{\mathbf{r}} f(\mathbf{r}, \tau) \frac{1}{\Psi_T(\mathbf{r})} \hat{\mathbf{H}} \Psi_T(\mathbf{r}) d\mathbf{r}}{\int_{\mathbf{r}} f(\mathbf{r}, \tau) d\mathbf{r}} = \frac{\langle \Phi(\tau) | \hat{\mathbf{H}} | \Psi_T \rangle}{\langle \Phi(\tau) | \Psi_T \rangle}, \quad (11)$$

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

The DMC energy corresponds to the following integral

$$E_{\text{DMC}} = \frac{\int_{\mathbf{r}} f(\mathbf{r}, \tau) \frac{1}{\Psi_T(\mathbf{r})} \hat{\mathbf{H}} \Psi_T(\mathbf{r}) d\mathbf{r}}{\int_{\mathbf{r}} f(\mathbf{r}, \tau) d\mathbf{r}} = \frac{\langle \Phi(\tau) | \hat{\mathbf{H}} | \Psi_T \rangle}{\langle \Phi(\tau) | \Psi_T \rangle}, \quad (11)$$

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

$$E_{\text{DMC}} = \frac{\langle \Phi(\tau) | E_0 | \Psi_T \rangle}{\langle \Phi(\tau) | \Psi_T \rangle} = E_0. \quad (12)$$

Limitations: VMC

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

Limitations: VMC

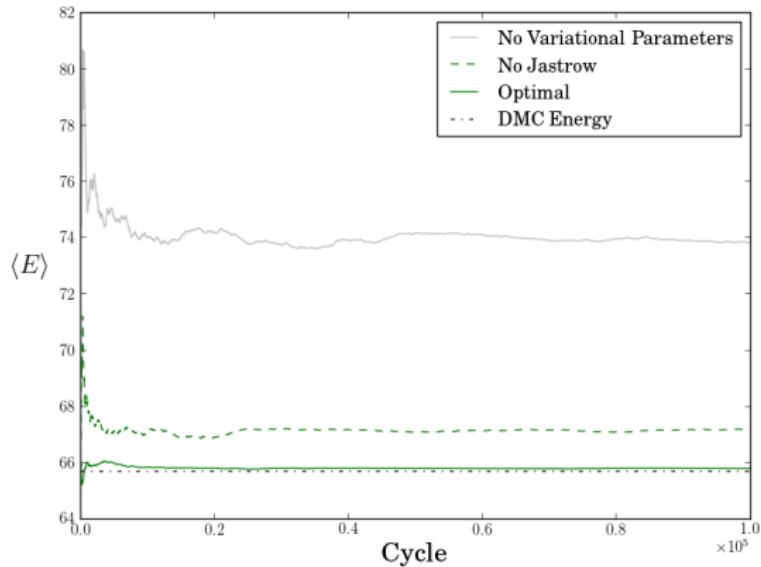


Figure: Comparison of different trial wave functions for a two-dimensional 12-particle quantum dot with unit frequency.

Limitations: DMC

As discussed previously: The fixed node approximation.

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Problem: The branching can get out of control for high *variance* systems.

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Solution: Can be countered by choosing a lower time step.

Consequence: Slower convergence. Breaking the requirement of *ergodicity*.

Limitations: DMC

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

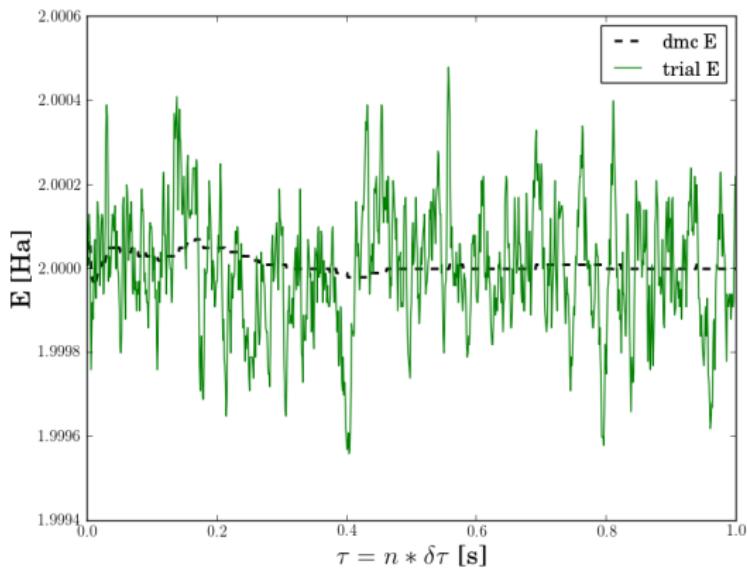
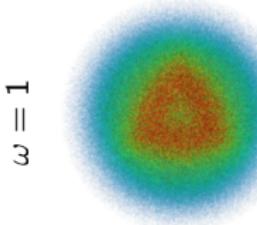


Figure: DMC calculation without the exact wave function. The exact result is $E_0 = 2$. The VMC energy is $2.0042(3)$, whereas the DMC energy is $2.00000(2)$.

Live demonstration



1
=

0.01
=

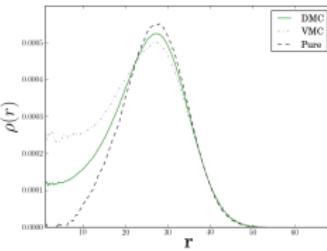
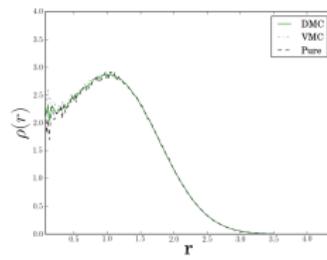
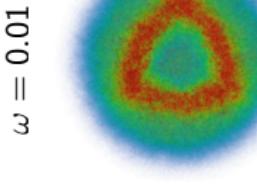


Figure: Demonstrated: Diffusion according to the following distributions.

The modelled systems

- Quantum dots
 - Two dimensions
 - Three dimensions
 - Double wells

The modelled systems

- Quantum dots
 - Two dimensions
 - Three dimensions
 - Double wells
- Atomic systems
 - Atoms
 - Homonuclear Diatomic Molecules

Quantum dots

Quantum dots are interacting electrons in a harmonic oscillator potential

$$V_{\text{ext}}(\mathbf{r}) = \frac{1}{2}\omega^2 r^2, \quad (13)$$

where ω is the oscillator frequency.

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where ω is the oscillator frequency.

The harmonic oscillator eigenfunctions are

$$\phi_{n_x, n_y, n_z}(\mathbf{r}) = H_{n_x}(\sqrt{\omega}x)H_{n_y}(\sqrt{\omega}y)H_{n_z}(\sqrt{\omega}z)e^{-\frac{1}{2}\omega r^2}, \quad (14)$$

where $H_n(x)$ is the n 'th level Hermite polynomial.

Quantum dots

Introducing a variational parameter α yields

$$\phi_{n_x, n_y, n_z}(\mathbf{r}; \alpha) = H_{n_x}(kx)H_{n_y}(ky)H_{n_z}(kz)e^{-\frac{1}{2}k^2r^2}, \quad (15)$$

where $k = \sqrt{\alpha\omega}$ represents the scaled oscillator potential.

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Solution: Quantum Monte-Carlo!

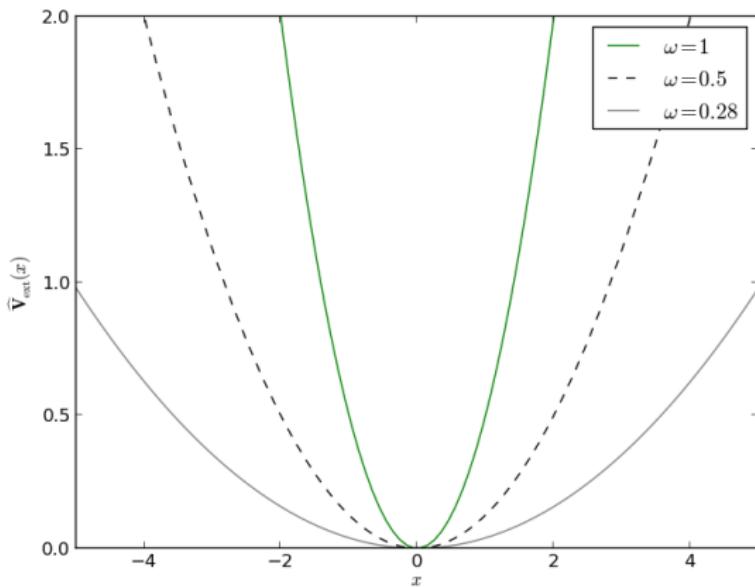


Figure: A one-dimensional version of the single-particle potential of quantum dots.

Double wells

The double-well potential used is

$$V_{\text{ext}}(\mathbf{r}) = \frac{1}{2}m^*\omega_0^2 \left[r^2 + \frac{1}{4}R^2 - R|x| \right], \quad (16)$$

where R is the well separation, and m^* and ω_0 are material constants.

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The construction of the new basis will be discussed later.

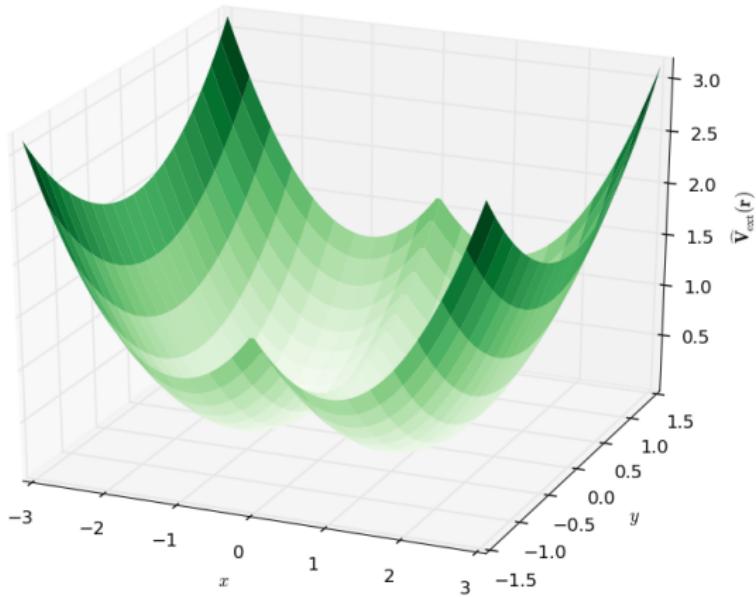


Figure: The external potential for a double-well quantum dot.

Atomic systems

Atomic systems are interacting electrons surrounding opposite charged nuclei. In the case of atoms, there is a single nucleus with charge $Z = N$. The potential used is

$$V_{\text{ext}}(\mathbf{r}) = -\frac{Z}{r}. \quad (17)$$

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This corresponds to the hydrogen atom potential with the *Born-Oppenheimer Approximation*.

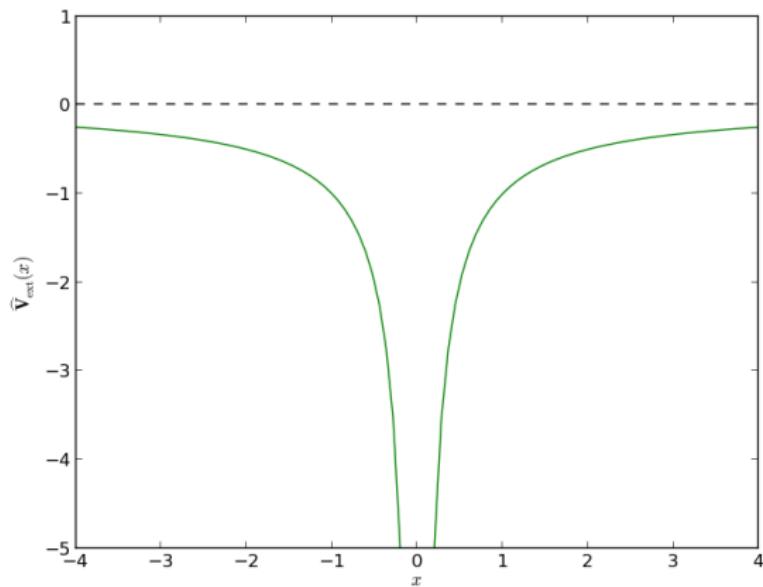


Figure: The one-dimensional version of the single-particle potential of hydrogen.

The eigenfunctions are

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

where $L_{q-p}^p(x)$ are the *associated Laguerre polynomials* and $Y_l^m(\theta, \phi)$ are the *spherical harmonics*.

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The spherical harmonics are related to the *associated Legendre functions* P_l^m in the following manner:

$$Y_l^m(\theta, \phi) \propto P_l^m(\cos \theta) e^{im\phi}. \quad (18)$$

Problem: The spherical harmonics are complex functions.

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Solution: Use a special superposition of spherical harmonics known as the real-valued *solid harmonics*

$$S_l^m(r, \theta, \phi) \propto r^l [Y_l^m(\theta, \phi) + (-1)^m Y_l^{-m}(\theta, \phi)] \quad (19)$$

$$\propto r^l P_l^{|m|}(\cos \theta) \begin{cases} \cos m\phi & m \geq 0 \\ \sin |m|\phi & m < 0 \end{cases}. \quad (20)$$

The resulting eigenfunctions become

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

where $k = \alpha Z$ is a scaled charge with α as a variational parameter.

Molecules

The Hamiltonian describing the homonuclear diatomic molecules is

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

where $Z = N/2$ is the charge of the nuclei, \mathbf{R} is the vector between the nuclei and \mathbf{r}_i is the coordinates of electron i .

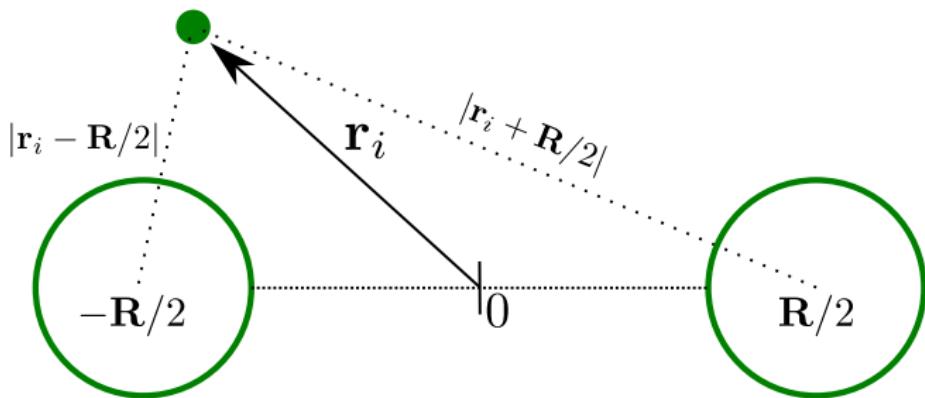


Figure: The model for the diatomic molecule.

In order to transform the hydrogen eigenstates $\phi_{nlm}^H(\mathbf{r})$, which are symmetric around a single nucleus, into molecular single-particle states $\phi_{nlm}^\pm(\mathbf{r}_i)$, a superposition of the two mono-nucleus wave functions are used:

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

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

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

ω	E _{VMC}	E _{DMC}	E _{FCI}
0.01	0.07406(5)	0.073839(2)	0.07383505
0.1	0.44130(5)	0.44079(1)	0.44079191
0.28	1.02215(5)	1.02164(1)	1.0216441
0.5	1.66021(5)	1.65977(1)	1.6597723
1.0	3.00030(5)	3.00000(1)	3.0000001

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

N	ω	E _{VMC}	E _{EDMC}	E _{SRG}	E _{CCSD}
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	ω	E _{VMC}	E _{DMC}	E ₀
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	2.000005(2)	2.000000(2)	2.0
	1.0	3.73032(8)	3.730123(3)	-
8	0.1	5.7130(6)	5.7028(1)	-
	0.28	12.2040(8)	12.1927(1)	-
	0.5	18.9750(7)	18.9611(1)	-
	1.0	32.6842(8)	32.6680(1)	-
20	0.1	27.316(2)	27.2717(2)	-
	0.28	56.440(2)	56.3868(2)	-
	0.5	85.714(2)	85.6555(2)	-
	1.0	142.951(2)	142.8875(2)	-

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

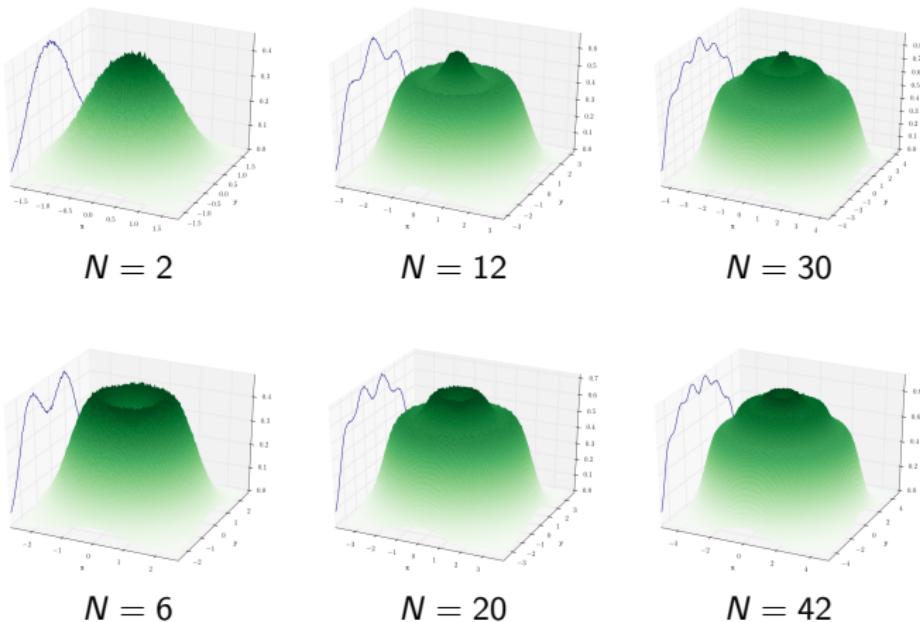


Figure: DMC one-body densities for two-dimensional quantum dots.

VMC density $|\Psi_T(\mathbf{r})|^2$

DMC density $\Phi(\mathbf{r}, \tau)\Psi_T(\mathbf{r})$

Pure density $|\Phi(\mathbf{r}, \tau)|^2$

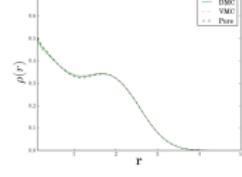
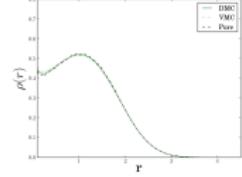
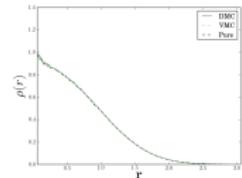
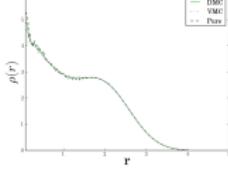
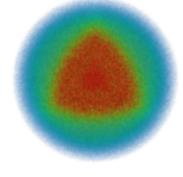
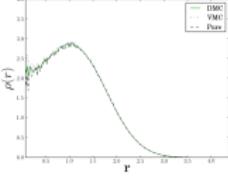
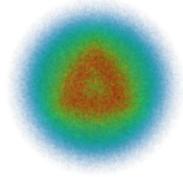
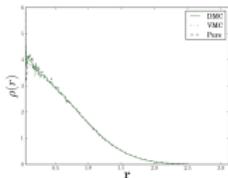
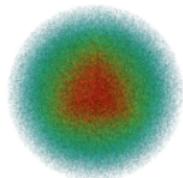
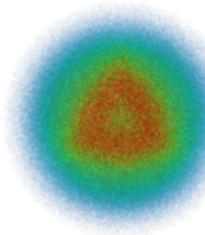


Figure: One-body densities for two- and three-dimensional quantum dots.

Lowering the frequency

1
||
3



0.01
||
3

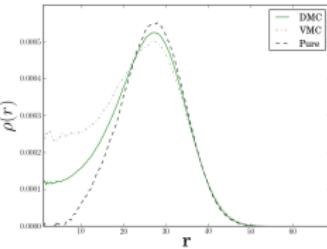
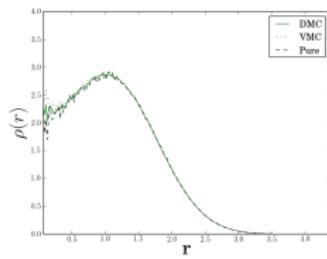
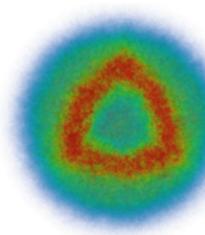
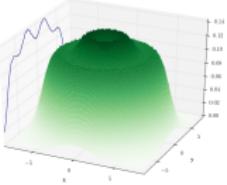
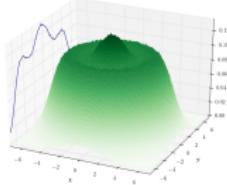
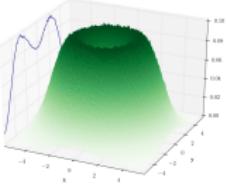
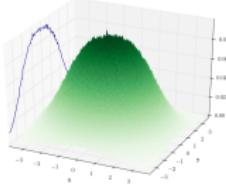
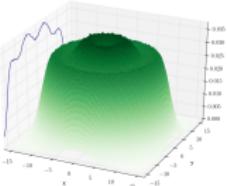
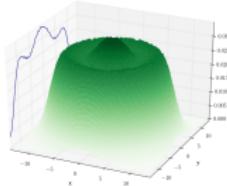
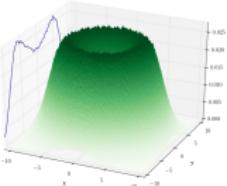
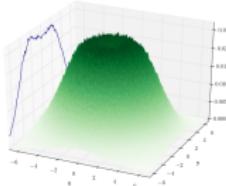


Figure: One-body densities for a 8-particle three-dimensional quantum dot for high and low frequencies.

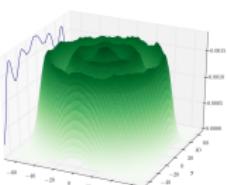
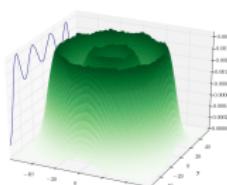
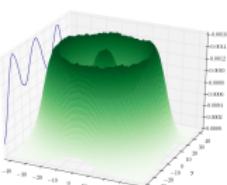
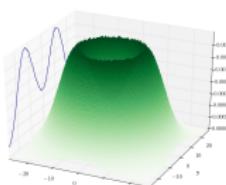
$\omega = 0.28$



$\omega = 0.1$



$\omega = 0.01$



$N = 2$

$N = 6$

$N = 12$

$N = 20$

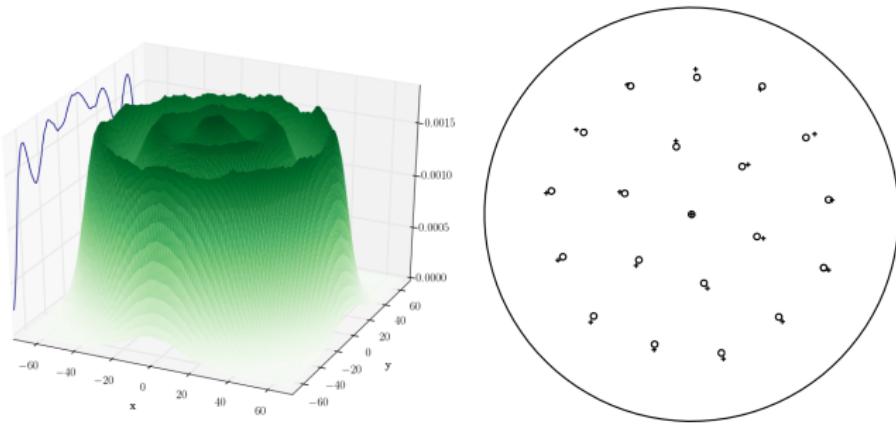


Figure: OBD for a 20-particle two-dimensional quantum dot compared to the classical theoretical configuration taken from P. Galatola et al. Eur. Phys. J. B **50**, 549 (2006)

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