Variational Reduced-Density-Matrix Theory Applied to the Hubbard Model

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Overview

1. Derivation of the variational approach
2. The N-representability problem
3. Constrained variational problem
4. Results for the 1D Hubbard model
5. Results for the 2D Hubbard model

The 1D results are from *Physical Review* **A73**, 062505 (2006).

Variational Theory

$$\hat{H} = \sum_{i,j} {}^1K^i_j \; \hat{a}^\dagger_i \hat{a}_j + \sum_{i,j,k,l} {}^2V^{i,j}_{k,l} \; \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}_l \hat{a}_k$$

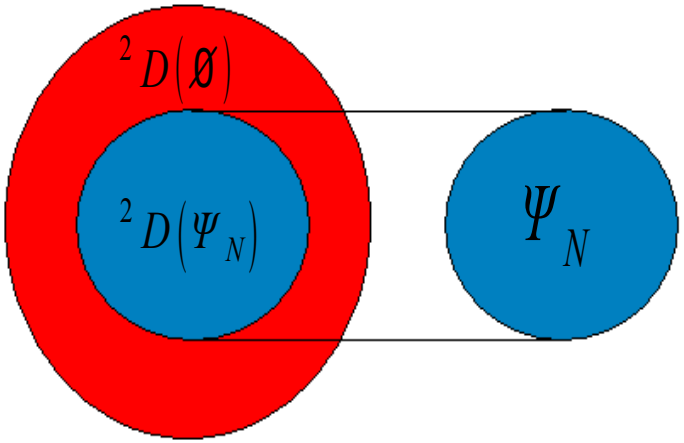
$$\begin{aligned}
E &= \langle \Psi | \hat{H} | \Psi \rangle \\
&= \sum_{i,j} {}^1K^i_j \langle \Psi | \hat{a}^\dagger_i \hat{a}_j | \Psi \rangle + \sum_{i,j,k,l} {}^2V^{i,j}_{k,l} \langle \Psi | \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}_l \hat{a}_k | \Psi \rangle \\
&= \sum_{i,j,k,l} {}^2K^{i,j}_{k,l} \langle \Psi | \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}_l \hat{a}_k | \Psi \rangle \\
&= \sum_{i,j,k,l} {}^2K^{i,j}_{k,l} {}^2D^{i,j}_{k,l}
\end{aligned}$$

N-Representability Problem

$$E = \min_{\Psi} \langle \Psi | \hat{H} | \Psi \rangle$$

$$E = \min_{\Psi} \mathrm{Tr}[{}^2K\,{}^2D]$$

$$E \neq \min_{{}^2D} \mathrm{Tr}[{}^2K\,{}^2D]$$



Reduced Density Matrices

$$^{1}D^{i}_{j} = \langle\psi|\hat{a}^{\dagger}_{i}\hat{a}_{j}|\psi\rangle$$

$$^{1}Q^{i}_{j} = \langle\psi|\hat{a}_{i}\hat{a}^{\dagger}_{j}|\psi\rangle$$

$$^{2}D^{i,j}_{k,l} = \langle\psi|\hat{a}^{\dagger}_{i}\hat{a}^{\dagger}_{j}\hat{a}_{l}\hat{a}_{k}|\psi\rangle$$

$$^{2}Q^{i,j}_{k,l} = \langle\psi|\hat{a}_{i}\hat{a}_{j}\hat{a}^{\dagger}_{l}\hat{a}^{\dagger}_{k}|\psi\rangle$$

$$^{2}G^{i,k}_{l,j} = \langle\psi|\hat{a}^{\dagger}_{i}\hat{a}_{k}\hat{a}^{\dagger}_{j}\hat{a}_{l}|\psi\rangle$$

$$^{3}D^{i,j,k}_{l,m,n} = \langle\psi|\hat{a}^{\dagger}_{i}\hat{a}^{\dagger}_{j}\hat{a}^{\dagger}_{k}\hat{a}_{n}\hat{a}_{m}\hat{a}_{l}|\psi\rangle$$

$$^{3}E^{i,j,k}_{l,m,n} = \langle\psi|\hat{a}^{\dagger}_{i}\hat{a}^{\dagger}_{j}\hat{a}_{k}\hat{a}^{\dagger}_{n}\hat{a}_{m}\hat{a}_{l}|\psi\rangle$$

$$^{3}F^{i,j,k}_{l,m,n} = \langle\psi|\hat{a}_{i}\hat{a}_{j}\hat{a}^{\dagger}_{k}\hat{a}_{n}\hat{a}^{\dagger}_{m}\hat{a}^{\dagger}_{l}|\psi\rangle$$

$$^{3}Q^{i,j,k}_{l,m,n} = \langle\psi|\hat{a}_{i}\hat{a}_{j}\hat{a}_{k}\hat{a}^{\dagger}_{n}\hat{a}^{\dagger}_{m}\hat{a}^{\dagger}_{l}|\psi\rangle$$

$$T_1 = {}^{3}D + {}^{3}Q$$

$$T_2 = {}^{3}E + {}^{3}F$$

Constrained Variational Problem

Enforcing antisymmetry and Hermiticity is trivial.

Positivity enforced through semidefinite programming.

Fixed trace, contraction relations between n- and (n+1)-RDMs, and mapping conditions between RDMs are constraints in the SDP.

Using SDP algorithm of Mazziotti reduces FP scaling to r^6 using matrix factorization (as opposed to r^{12} in primal-dual methods). The bottleneck is DGEMM on the largest density matrix block.

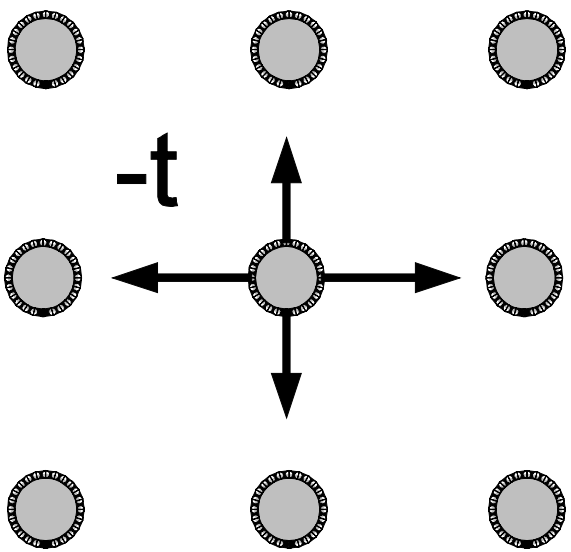
Details are available in many of our papers. You can link to all of them from http://mazziotti.uchicago.edu.

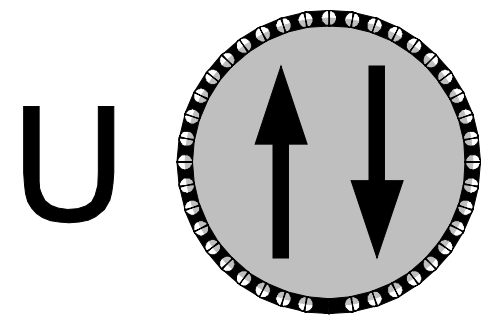
Why Physicists Might Like It

- Variational lower bound
- Does not suffer from orbital order problems like DMRG, indifferent to dimensionality
- Polynomial scaling, very low memory requirements
- Non-perturbative – never blows up, no need to partition Hamiltonian
- Straightforward treatment of all symmetries: SO(4), C_{4v}, T_x
- Valid for bosons, fermions and mixtures thereof
- Immediately generates all 1,2-RDMs including off-diagonal matrix elements: correlation functions & ODLRO

The Hubbard Model

$$\hat{H} = -t \sum_{\langle ij \rangle, \sigma} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + U \sum_{i} \left(\hat{c}^{\dagger}_{i,\alpha} \hat{c}_{i,\alpha} - \frac{1}{2} \right) \left(\hat{c}^{\dagger}_{i,\beta} \hat{c}_{i,\beta} - \frac{1}{2} \right)$$





Spin Symmetries

$$ {}^2D^{i_\alpha j_\beta}_{k_\alpha, l_\beta} \rightarrow \begin{pmatrix} {}^2D^{i_\alpha j_\beta + j_\alpha i_\beta}_{k_\alpha l_\beta + l_\alpha k_\beta} & 0 \\ 0 & {}^2D^{i_\alpha j_\beta - j_\alpha i_\beta}_{k_\alpha l_\beta - l_\alpha k_\beta} \end{pmatrix} = \begin{pmatrix} {}^2D^{S=0}_{ij,kl} & 0 \\ 0 & {}^2D^{S=1}_{ij,kl} \end{pmatrix} $$

Full SO(4) is straightforward but isn't in the code at the moment

Finite magnetization reduces SU(2) to U(1) in spin

Finite chemical potential reduces SU(2) to U(1) in pseudospin

Either SU(2) only reduces the rank of the 2-RDMs by a factor of two but enforcing SU(2) spin on singlets increases accuracy

Lattice Symmetries

$SU(2)$

Lattice	1-RDM	2-RDM	3-RDM	Count
4×4	16	256	4096	2
6×6	36	1296	46656	2
8×8	64	4096	262144	2
10×10	100	10000	1000000	2
$L \times L$	L^2	L^4	L^6	2

$SU(2) \otimes T_x \otimes T_y$

Lattice	1-RDM	2-RDM	3-RDM	Count
4×4	1	16	256	16
6×6	1	36	1296	36
8×8	1	64	4096	64
10×10	1	100	10000	100
$L \times L$	1	L^2	L^4	L^2

Accuracy of Energy

	FCI		DQG		DQGT	
U	E_{FCI}	E_{CORR}	$E_{\mathrm{RDM}} - E_{\mathrm{FCI}}$	$\%E_{\mathrm{CORR}}$	$E_{\mathrm{RDM}} - E_{\mathrm{FCI}}$	$\%E_{\mathrm{CORR}}$
1	-6.601	-0.203	-0.0161	107.94	-0.0006	100.30
2	-5.409	-0.830	-0.0669	108.06	-0.0046	100.55
3	-4.433	-1.897	-0.1401	107.39	-0.0150	100.79
4	-3.669	-3.334	-0.2094	106.28	-0.0212	100.63
8	-2.048	-10.122	-0.2999	102.96	-0.0338	100.33
20	-0.853	-29.163	-0.1870	100.64	-0.0160	100.05
40	-0.429	-59.573	-0.1009	100.17	-0.0064	100.01
80	-0.215	-119.785	-0.0514	100.04	-0.0016	100.00

E_{CORR} is the energy from the connected 2-RDM (cumulant).

The details are in the paper.

Accuracy of 2-RDM

	Antisymmetric			Symmetric		
		$\|^2 D_{\mathrm{RDM}} - {}^2 D_{\mathrm{FCI}}\|_2$			$\|^2 D_{\mathrm{RDM}} - {}^2 D_{\mathrm{FCI}}\|_2$	
U	$\|^2 D_{\mathrm{FCI}}\|_2$	DQG	DQGT	$\|^2 D_{\mathrm{FCI}}\|_2$	DQG	DQGT
1	0.9873	0.0039	0.0010	1.0042	0.0199	0.0049
2	0.9482	0.0137	0.0030	1.0056	0.0410	0.0044
3	0.8834	0.0225	0.0051	0.9910	0.0722	0.0163
4	0.8026	0.0344	0.0088	0.9589	0.1127	0.0241
8	0.5543	0.0641	0.0074	0.8265	0.2056	0.0166
20	0.3798	0.0921	0.0093	0.7383	0.2782	0.0252
40	0.3372	0.0969	0.0078	0.7226	0.2913	0.0204
80	0.3241	0.0981	0.0082	0.7185	0.2946	0.0208

Larger Lattices

	$\lvert\Lambda\rvert = 10$			$\lvert\Lambda\rvert = 14$		
	E_{Exact}	Error per site		E_{Exact}	Error per site	
U	per site	DQG	DQGT	per site	DQG	DQGT
1	-1.0614	-0.0040	-0.0002	-1.0511	-0.0046	-0.0004
2	-0.8638	-0.0162	-0.0009	-0.8539	-0.0185	-0.0024
3	-0.7046	-0.0326	-0.0021	-0.6963	-0.0362	-0.0041
4	-0.5834	-0.0458	-0.0052	-0.5777	-0.0491	-0.0077
5	-0.4933	-0.0533	-0.0075	-0.4895	-0.0561	-0.0094
6	-0.4255	-0.0568	-0.0085	-0.4226	-0.0594	-0.0099
7	-0.3730	-0.0579	-0.0085	-0.3707	-0.0603	-0.0097
8	-0.3315	-0.0576	-0.0082	-0.3295	-0.0599	-0.0089
10	-0.2704	-0.0547	-0.0069	-0.2688	-0.0570	-0.0074
20	-0.1390	-0.0372	-0.0027	-0.1381	-0.0391	-0.0028
100	-0.0281	-0.0087	-0.0002	-0.0279	-0.0093	-0.0001

Preliminary Results for 2D

4x4	U = 1	U = 4
DQG	-20.958	-14.945
DQGT	-20.844	TBA
EXACT	-20.794	-13.622

10x10 lattice at DQG requires less than 400 MB RAM

High-spin states can be done with minor modification, triplets were done for 1D Hubbard already

DMRG/VRDM would give upper/lower bounds

Including the 3-cumulant ($^3D/^3E/^3F/^3Q$ vs. T_1/T_2) should increase accuracy an order of magnitude

Pre-empting Questions

- What about excited states, Green's function, etc.?

  Excited-states of different symmetry are trivial; other excited states can be obtained (see papers) but we have tested the accuracy yet.

- What about other models besides the Hubbard?

  We don't exploit any of the simplicity of the t-U form; can do the t-t'-t''-t'''...-U-V-W-X-Y-Z... Hubbard model. Can couple to bosons ala Hubbard-Holstein as well.

- Can we study superconductivity with RDM method?

  I haven't looked for it yet, but feel free to email me suggestions. Calculations are done at T=0 and we do not yet have a way to calculate the order parameter: $\langle\psi|\hat{a}_i^\dagger\hat{a}_j^\dagger|\psi\rangle$

Acknowledgements

David is giving a talk next door in about an hour
if you want to hear more about RDM methods.

Thanks to: Eugene Kamarchik, University of Chicago

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Demonstrated Applications

- **Excited-states and ionization energies:** D. A. Mazziotti, *Phys. Rev. A* **68**, 052501 (2003) and J. D. Farnum and DAM, *Chem. Phys. Lett.* **400**, 90 (2004).
- **Open-shell molecules:** JRH and DAM, *Phys. Rev. A* **73**, 012509 (2006).
- **Strong electric fields:** G. Gidofalvi and DAM, *J. Phys. Chem. A.* **110**, 5481 (2006) and JDF, GG and DAM, *J. Chem. Phys.* **124**, 234103 (2006).
- **Geometry optimization of small clusters:** E. Kamarchik and DAM, *Phys. Rev. A* **75**, 013203 (2007).
- **Non-Born-Oppenheimer calculations:** EK and DAM, work in-progress.
- **Sage model:** GG and DAM, *Phys. Rev. A* **69**, 042511 (2004).
- **Lipkin model of nuclear correlations:** JRH and DAM, *Phys. Rev. A* **71**, 062503 (2005) and others.
- **Quantum phase transitions:** GG and DAM, *Phys. Rev. A* **74**, 012501 (2006).
- **1D Hubbard:** JRH and DAM, *Phys. Rev. A* **73**, 062505 (2006).
- **2D Hubbard:** JRH and DAM, work in-progress.