Variational quantum dynamics

Joachim Brand

Massey University, New Zealand

Lecture IV - Victorian Summer School in Ultracold Physics (VSSUP) 2012

"Since the fabric of the Universe is most perfect and is the work of a most wise Creator, nothing whatsoever takes place in the Universe in which some relation of maximum and minimum does not appear."

Leonard Euler

Variational principle in classical mechanics

- Hamilton's principle (stationary action principle):
  - classical action

$$\mathcal{S}[\mathbf{q}] \stackrel{\text{def}}{=} \int_{t_1}^{t_2} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\, dt$$

  - Variation with respect to the trajectory function

$$\frac{\delta \mathcal{S}}{\delta \mathbf{q}(t)} = 0$$

  - Leads to the Euler-Lagrange equations (and classical mechanics)

$$\frac{\partial L}{\partial \mathbf{q}} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\mathbf{q}}} = 0$$

Variational principle in quantum mechanics

- Find approximate ground state by minimizing

$$\varepsilon[\Psi] = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}.$$

- Unrestricted variation yields the Schrödinger equation

$$\frac{\delta \varepsilon}{\delta \Psi^*} = 0 \quad \longrightarrow H|\Psi\rangle = \varepsilon|\Psi\rangle$$

- As an approximation method, we choose a physically reasonable ansatz to parameterize the wave function $\Psi[\lambda_1, \ldots]$ and solve $\dfrac{\partial \varepsilon}{\partial \lambda_i} = 0$

- Any approximate solution yields an upper bound to the ground state energy and is 'optimal' as it is the minimum possible in the variational space $\varepsilon[\Psi'] \geq E_0$

Constraints

- Often we may want to introduce constraints to the wave function, e.g. normalization or orthogonality conditions of the type $\eta[\Psi] = n$
- Here the method of undetermined Lagrange multipliers is useful
- Instead of $\varepsilon[\Psi]$ we vary

$$L[\Psi] = \varepsilon[\Psi] - \lambda(\eta[\Psi] - n)$$

where λ is the Lagrange multiplier

- Variation

$$\delta L = \delta\varepsilon - \lambda\delta\eta$$

leads to a wave function that depends on Lagrange multiplier (this can later be determined)

$$\Psi(\lambda)$$

Example: single mode

- We choose $|\Psi\rangle = \frac{1}{\sqrt{N!}}(a^\dagger)^N|\mathrm{vac}\rangle$

  and perform a variation with respect to the mode function

  $$\phi(x) = [\psi(x), a^\dagger] \qquad a^\dagger = \int d^D x\ \phi(x)\psi^\dagger(x)$$

  with a constraint to ensure normalization of the mode function $\varepsilon[\phi] = \langle\Psi|H|\Psi\rangle - \mu N(\int \phi^*(x)\phi(x)d^D x - 1)$

  with $H = \int d^D x\ \psi^\dagger(x)h_1\psi(x) + \frac{g}{2}\int d^D x\ \psi^\dagger(x)\psi^\dagger(x)\psi(x)\psi(x)$

- What do we obtain?

  The GP equation! $\mu\phi(x) = h_1\phi(x) + g(N-1)|\phi(x)|^2\phi(x)$

Single configuration methods (self consistent field)

- Hartree product
  (distinguishable particles)
  $$\Psi(x_1, x_2, \ldots) = \phi_1(x_1)\phi_2(x_2)\cdots$$

- Identical Hartree product
  GP equation
  $$\frac{1}{\sqrt{N!}}(a^\dagger)^N|\mathrm{vac}\rangle \leftrightarrow \phi(x_1)\phi(x_2)\cdots$$

- Permanent (symmetrised product)
  Best mean field – Hartree Fock (Bosons)
  $$(a_1^\dagger)^{N_1}(a_2^\dagger)^{N_2}\cdots|\mathrm{vac}\rangle \leftrightarrow \mathcal{S}\{\phi_1(x_1)\phi_1(x_2)\cdots\}$$
- Slater determinant: Hartree-Fock method (Fermions)
  $$c_1^\dagger c_2^\dagger \cdots c_N^\dagger|\mathrm{vac}\rangle \leftrightarrow \mathcal{A}\{\phi_1(x_1)\phi_2(x_2)\cdots\}$$

Variation is performed wrt the orbital functions.
This leads to nonlinear (self-consistent) equation

What about an expansion in permanents?

- i.e. expand in an occupation number basis

$$|\Psi\rangle = \sum_J C_J |J\rangle \qquad\qquad |J\rangle = \bar{N}(a_1^\dagger)^{N_1}(a_2^\dagger)^{N_2}\cdots|\mathrm{vac}\rangle$$

- Variation with respect to coefficients:
  - Leads to matrix eigenvalue equation
  - This is known as “exact diagonalisation” or “full CI (configuration interaction)”
  - Hard to do if you have large basis or many particles
- Variation with respect to orbitals and coefficients:
  - This is known as multi-configurational SCF method
  - Need a smaller set of orbitals (matrix dimension)
  - One of the most accurate methods of Quantum Chemistry

Time-dependent variational principles

- Stationary action principle

$$\delta S = 0 \qquad\qquad S = \int_{t_1}^{t_2} dt\ \langle \Psi | H - i\hbar\partial_t | \Psi \rangle$$

- Dirac-Frenkel variational principle

$$\langle \delta\Psi | H - i\hbar\partial_t | \Psi \rangle = 0$$

- McLachlan variational principle

$$||i\hbar\theta - H\Psi||^2 = \mathrm{Min} \qquad\qquad \theta = \dot{\Psi}$$

It turns out, these are all equivalent if variation is performed wrt complex parameters
(see Kucar, 1987, and Beck 2000, p113)

Ideology of variational quantum dynamics

- Variational derivation of GP function interprets the GP order parameter as a single-particle or “mode” function that describes the motion of a single-particle in a many particle environment (involving lots of “elementary modes” or “primitive basis functions”).
- Systematic improvement upon GP is found by allowing superpositions of permanents, i.e. correlation.
- There is no notion of quantum or thermal “noise” in this formulation. Finite temperature would have to be treated by explicit ensemble averaging.
- The actual many-body wave function (at the given level of approximation) is available.

Multi-configurational time-dependent Hartree for bosons (MCTDH-B)

- Start with a basis of *permanents* (i.e. symmetrised products)
- Best written in second quantisation (occupation number basis)

$$|\Psi(t)\rangle = \sum_{\vec{n}} C_{\vec{n}}(t)|\vec{n};t\rangle,$$

$$|\vec{n};t\rangle = \frac{1}{\sqrt{n_1!n_2!n_3!\cdots n_M!}} \times [b_1^\dagger(t)]^{n_1}[b_2^\dagger(t)]^{n_2}\cdots[b_M^\dagger(t)]^{n_M}|\mathrm{vac}\rangle$$

MCTDH-B equations of motion

- Variation of the time-dependent coefficient vector and mode/single-particle functions leads to coupled equations of motion

$$i|\dot{\phi}_j\rangle = \hat{\mathbf{P}}\left[\hat{h}|\phi_j\rangle + \sum_{k,s,q,l=1}^{M} \{\boldsymbol{\rho}(t)\}^{-1}_{jk}\rho_{ksql}\hat{W}_{sl}|\phi_q\rangle\right]$$

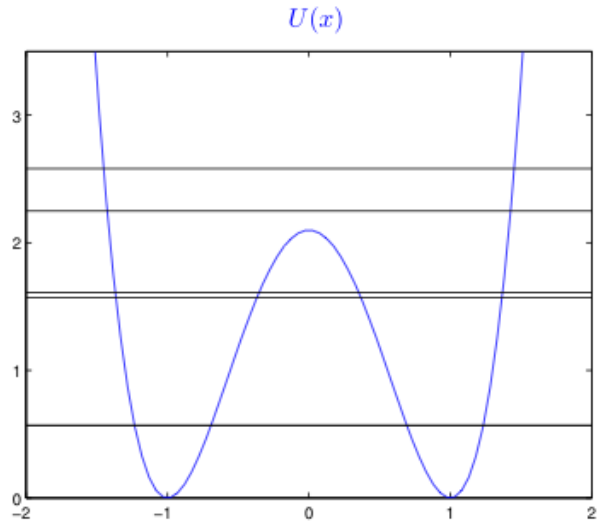
$$\hat{\mathbf{P}} = 1 - \sum_{j'=1}^{M} |\phi_{j'}\rangle\langle\phi_{j'}|.$$

$$\mathbf{H}(t)\mathbf{C}(t) = i\frac{\partial \mathbf{C}(t)}{\partial t}$$

$$H_{\vec{n}\vec{n}'}(t) = \langle \vec{n}; t|\hat{H}|\vec{n}'; t\rangle$$

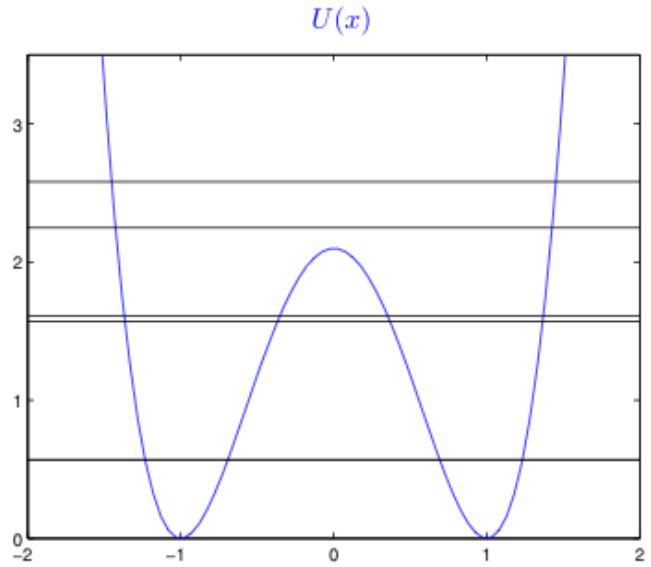
Example: Double well, levels of approximation

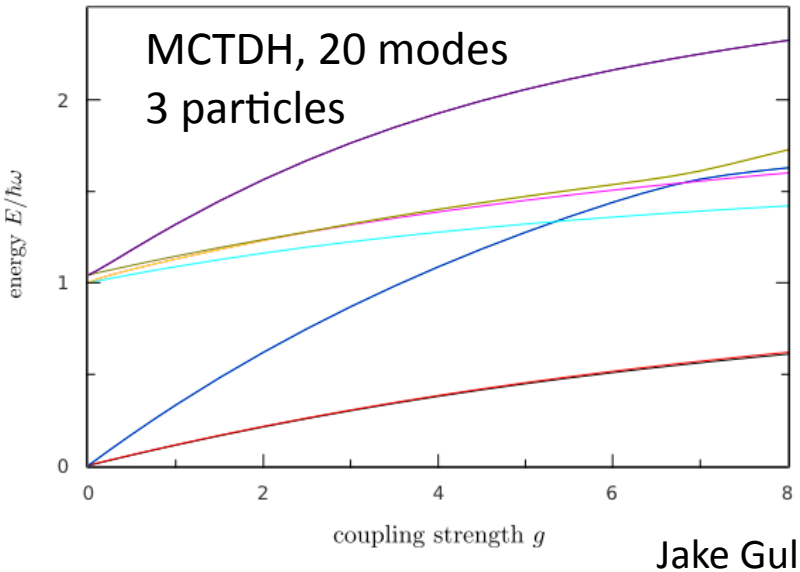
- Hierarchy of two-mode approximations:
  1. 2 mode Gross-Pitaevskii (project GP onto two *rigid* modes), gives classical pendulum equation
  2. 2 mode Bose-Hubbard (or Lipkin-Meshkov-Glick), full quantum model with 2 modes
  3. 2 mode MCTDH-B: As in 2. but with variationally optimised "modes" that can distort due to particle interaction, can take into account some features of upper excitation bands

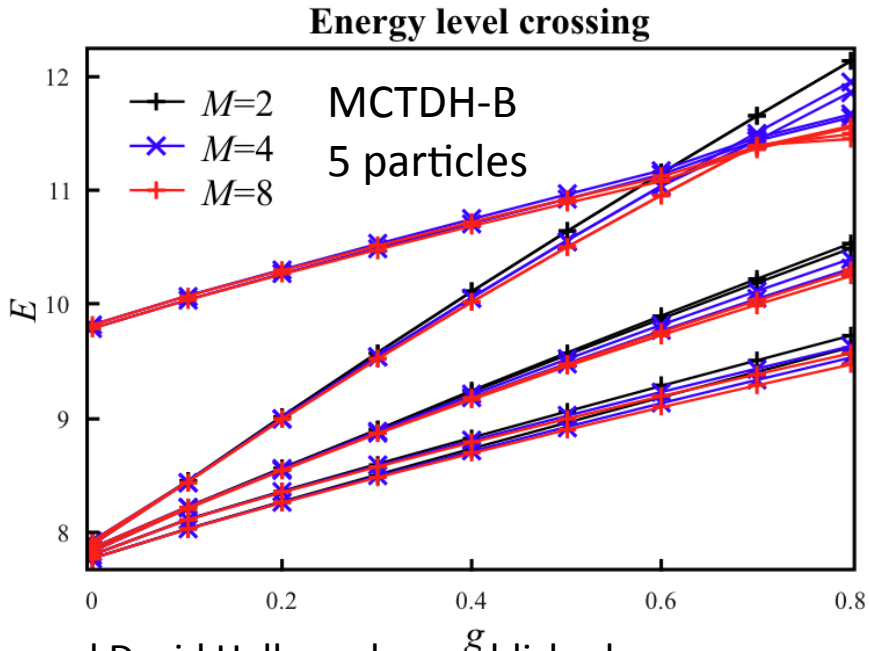


Example: double well

- MCTDH can be compared to a two-site Bose-Hubbard (or Lipkin-Meshkov-Glick) model.
- In LMG, the excited state energies are (almost) linear with g. MCTDH can capture the non-linearity.







Jake Gulliksen and David Hallwood, unpublished

Derivation of MCTDH-B

- Use least action principle (or Dirac-Frenkel)
- Use Lagrange multipliers (LM) to ensure orthogonality and normalization of single-particle functions (spfs)

$$S[\{C_{\vec{n}}(t)\},\{\phi_k(\mathbf{r},t)\}] = \int dt \left\{ \langle \Psi | \hat{H} - i\frac{\partial}{\partial t} | \Psi \rangle \; - \sum_{k,j=1}^{M} \mu_{kj}(t)[\langle \phi_k | \phi_j \rangle - \delta_{kj}] \right\}.$$

- Vary *S* with respect to spfs and coefficient vector.
- Make use of ambiguity of representation (unitary transformations in single-particle space) to simplify equations

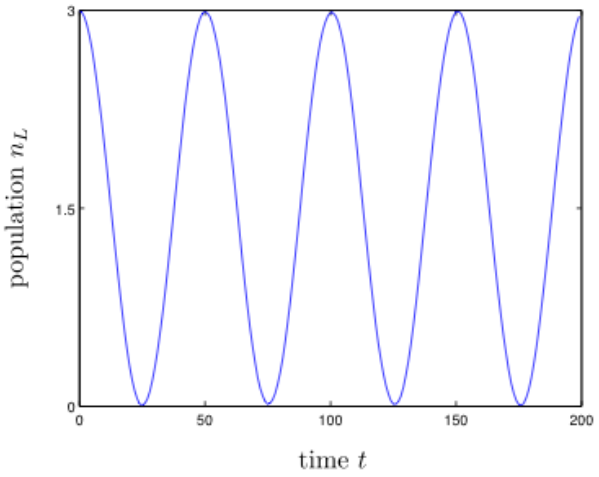
$$\langle \phi_k | \dot{\phi}_q \rangle = 0, \quad k,q = 1, \ldots, M$$

- Eliminate LMs in favour of projection operators
- Resulting equations of motion conserve energy, normalization and orthogonality of the single-particle functions

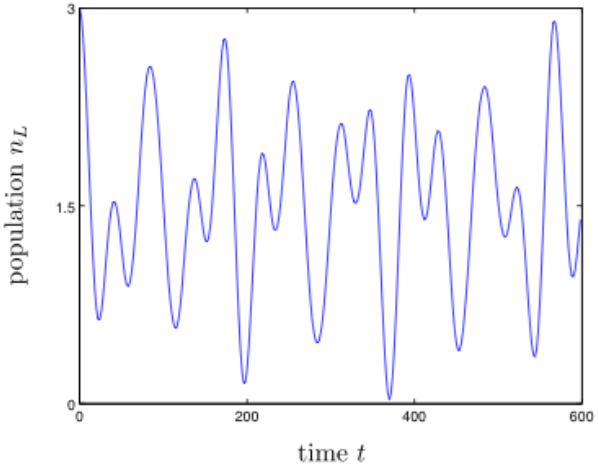
Why time dependence?

- Wave function is represented by (large) vector. The Hamiltonian is a (sparse) matrix. Time propagation is based on matrix-vector multiplication $O(n^2)$.
- Diagonalization of the matrix is $O(n^3)$ – more expensive.
- Ground and excited states can be calculated using imaginary-time propagation (relaxation) and combination of relaxation and diagonalization of coefficient matrix.
- It's cool to study dynamics!

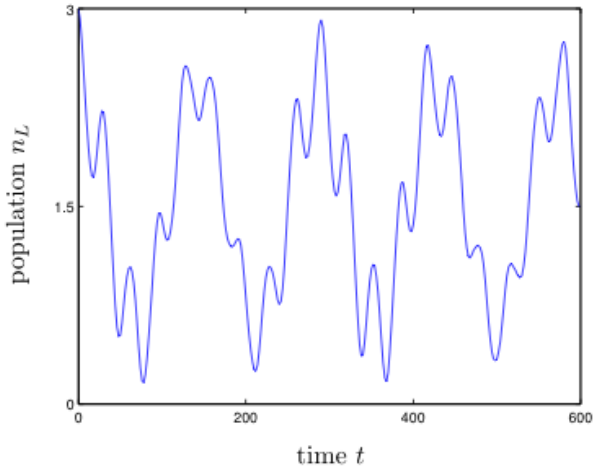
Quantum dynamics with 3 particles in 20 modes

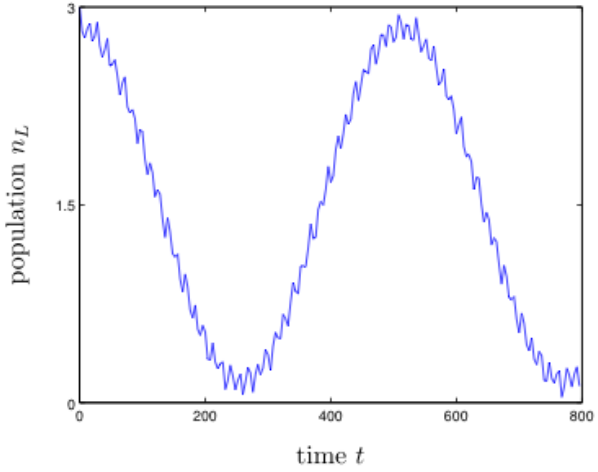


(a)



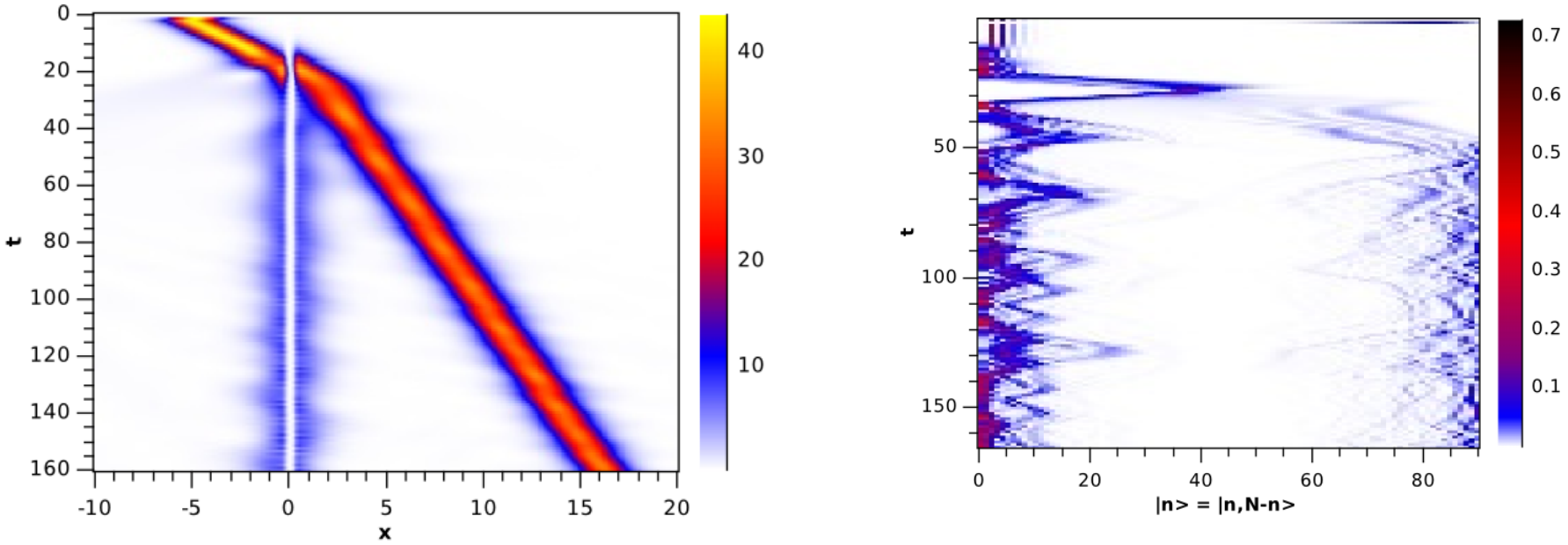
(b)





Jake Gulliksen, MSc thesis (unpublished)

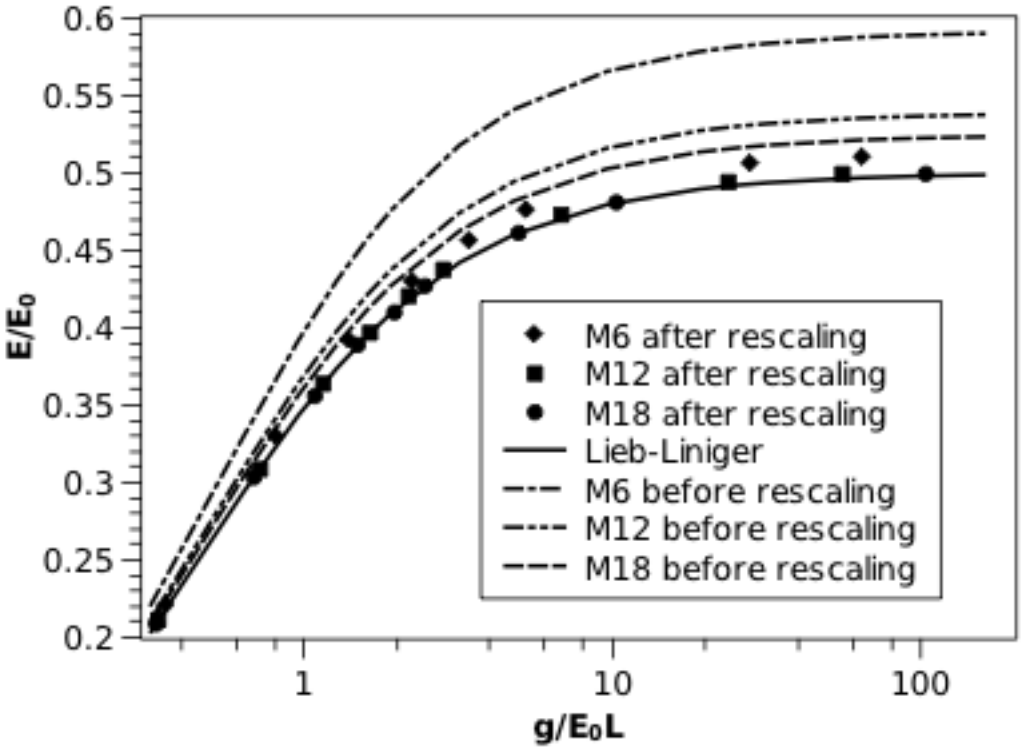
And with 90 particles in 2 modes



Thomas Ernst (unpublished)

What about strong interactions?

- Can we treat the physics of the Lieb-Liniger model and Tonks-Girardeau gas with these methods?
- This is hard because the number of modes involved becomes huge – truncation introduces significant errors!
- Lieb-Linger exact solutions provide an excellent bench-mark.



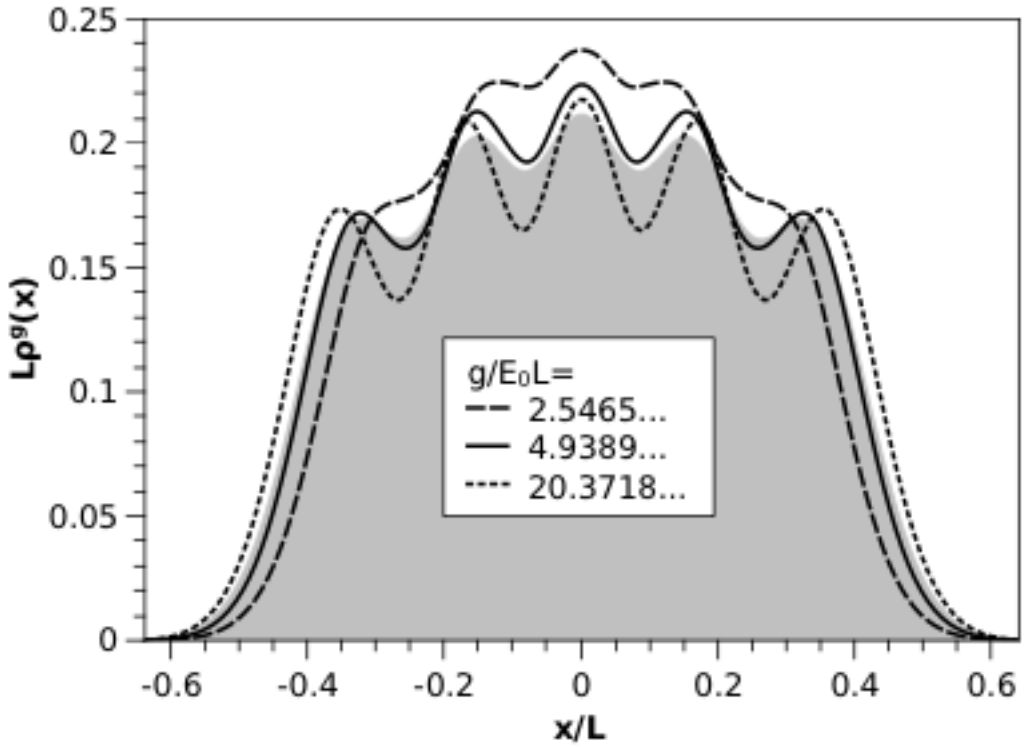
Rescaling

- Simple rescaling of the interaction strength can greatly reduce the basis set truncation error in finite calculations.
- This has been shown to be exact for 2 particles in a ring geometry.
- Empirical evidence with up to five particles and in harmonic and double well potentials (with MCTDH) supports rescaling as a general method to reduce errors.

Hallwood, Ernst, Brand (2010)

Ernst, Hallwood, Gulliksen, Meyer, Brand (2011)

Density of Tonks-Girardeau state in harmonic trap



Density of five particles in harmonic trap at TG limit (grey) and with MCTDH (13 modes) at different interaction strengths.
The full line is the rescaled result.

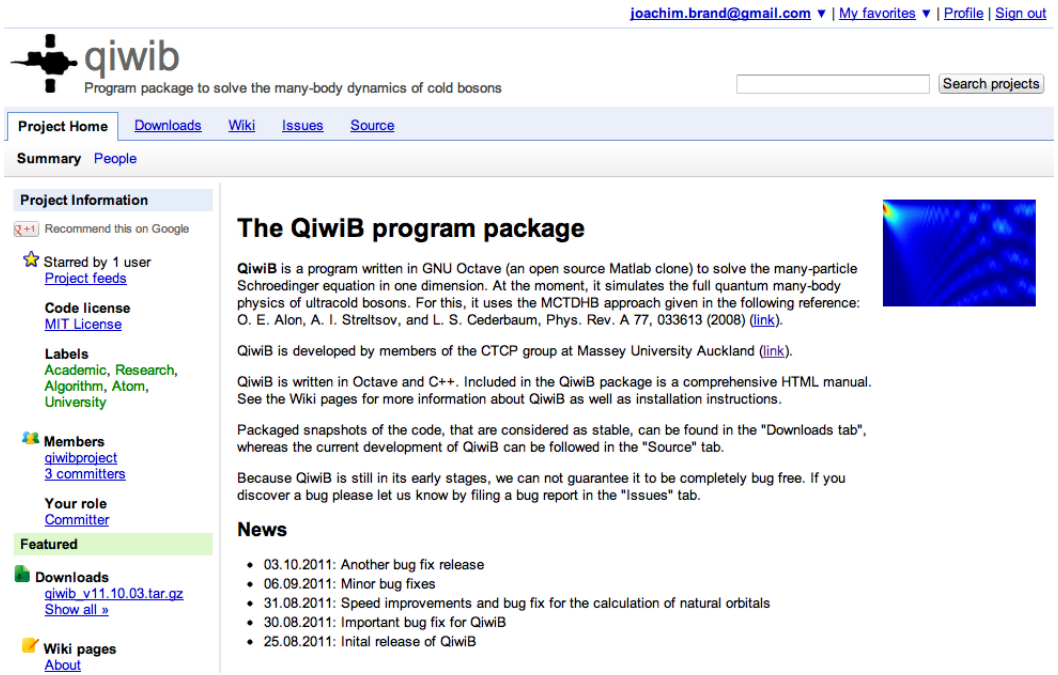
Ernst, Hallwood, Gulliksen, Meyer, Brand (2011)

Flavours and history

- MCTDH (distinguishable particles) goes back to 1992 publication
  - Big package, maintained by Hans-Dieter Meyer, distributed to all who ask, mailing list, regular releases
  - Mainly used for quantum molecular dynamics, i.e. chemical reactions, molecular vibration and dissociation
  - Forks and different version of code exist in many places in the world
  - Used for cold atoms
- MCTDH-F
  - Coded by 3 different groups
  - Used for electron dynamics in strong fields; not yet applied to ultra-cold atoms
- MCTDH-B
  - Most efficient for boson problems
  - Two implementations exist:
    - Heidelberg: Streltsov, Alon, Cederbaum
    - Auckland (QiwiB)

QiwiB (Quantum integrator with interacting bosons)

- Open source package to solve the MCTDH-B equations
- To study quantum dynamics of single-component Bose systems in one dimension
- Extension to multi-component systems is under way
- Developed by Thomas Ernst with contributions from D.W. Hallwood, J. Brand, J. Avery (extension)
- Easy to install under linux / MacOsX, requires Octave and open source libraries
- Available at code.google.com/p/qiwib



Bibliography

- MCTDH (Heidelberg) package web page: **http://www.pci.uni-heidelberg.de/cms/mctdh.html**
- **QiwiB** (Auckland) package web page: http://code.google.com/p/qiwib/
- ***Multidimensional Quantum Dynamics: MCTDH Theory and Applications*** H.-D. Meyer, F. Gatti, and G. A. Worth, editors, books.google.com
- Multiconfigurational time-dependent Hartree method for bosons: Many-body dynamics of bosonic systems, Ofir E. Alon, Alexej I. Streltsov, and Lorenz S. Cederbaum, Phys. Rev. A **77**, 033613 (2008)
- Best mean field for condensates, L. S. Cederbaum and A. I. Streltsov, Phys. Lett. A **318**, 564 (2003)
- M. H. Beck, A. Jäckle, G. A. Worth and H.-D. Meyer. *The multiconfiguration time-dependent Hartree method: A highly efficient algorithm for propagating wavepackets.* Physics Reports **324** (2000), 1 [pdf download].
- J. Kucar, H.-D. Meyer, and L. Cederbaum, Chem. Phys. Lett. 140, 525 (1987).
- **Robust Mesoscopic Superposition of Strongly Correlated Ultracold Atoms** D. W. Hallwood, T. Ernst, J. Brand, *Phys. Rev. A* **82**, 063623 (2010)
- **Simulating strongly correlated multiparticle systems in a truncated Hilbert space**, T. Ernst, D. W. Hallwood, J. Gulliksen, H.-D. Meyer, J. Brand, Phys. Rev. A 84, 023623 (2011)