Supercomputing tool for superfluid systems

TAPIO SIMULA AND KAZUSHIGE MACHIDA







Outline

- ✓ Solved problems
 - Bragg scattering a vortex state
 - Vortex waves
- ✓ Methodology $δ_{\alpha\beta}$
- $u_{\alpha}(x_{\beta}) = \sqrt{w_{\alpha}}$ V Problems to be solved

Archimede's quantum screw

light-shift potential from Laguerre+Gaussian laser fields

 $V_{\rm ext}(\mathbf{r},t) = |A_{\rm G}|^2 + |A_{\rm LG}|^2 + 2A_{\rm G}^*A_{\rm LG}\cos(2kz + \Delta\omega t + \phi)$



Quantized Rotation of Atoms from Photons with Orbital Angular Momentum

M. F. Andersen, C. Ryu, Pierre Cladé, Vasant Natarajan,^{*} A. Vaziri,[†] K. Helmerson, and W. D. Phillips Atomic Physics Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899-8424, USA (Received 26 June 2006; published 26 October 2006)

T. P. Simula, N. Nygaard, S. X. Hu, L.A. Collins, B. I. Schneider, and K. Mølmer, Phys. Rev. A 77, 015401 (2008)





Quadrupole Oscillation of a Single-Vortex Bose-Einstein Condensate: Evidence for Kelvin Modes







 $V_{\text{pert}}(\mathbf{r},t) = \epsilon m \omega_{\perp}^2 \cos(\Omega t) \cos(\mathbf{k}_z z) (x^2 + y^2)$



t = 0 ms



T. P. Simula, T. Mizushima, and K. Machida, PRA (2008)



Kelvin-Tkachenko modes



work in progress



Time = 0



Column









Time = 0.0796





Slice



Time = 0



Column





Methodology (3, 0.6)

✓ Discrete Variable Representation^{-0.2}

- "massaged" polynomial basis (Hermite, Legendre, Laguerre...)
- quadrature rule $\langle f|g \rangle \equiv \int_{a}^{b} dx \, w(x) f(x) g(x) \approx \sum_{\alpha=1}^{N} w_{\alpha} f(x_{\alpha}) g(x_{\alpha})$ • DVR basis functions $u_{\alpha}(x_{\beta}) = \frac{\delta_{\alpha\beta}}{\sqrt{w_{\alpha}}}$ weights

0.8

 $\{\phi_n, n = 0, \dots, N - 1\}$

• diagonal potential operator $\langle u_{\alpha}|\hat{x}|u_{\beta}\rangle = \sum w_{q}u_{\alpha}^{*}(x_{q})x_{q}u_{\beta}(x_{q}) = x_{\alpha}\delta_{\alpha\beta}$



• very sparse matrix representation



- efficient temporal propagation (TDGPE) $e^{-iH\Delta t/\hbar} \approx e^{-iV\Delta t/2\hbar} e^{-iT\Delta t/\hbar} e^{-iV\Delta t/2\hbar}$
- scalable parallelization using MPI



-X

X

✓ parallelized diagonalization of large matrices

Bogoliubov-de Gennes equations for Bose and Fermi systems

$$\begin{pmatrix} \mathcal{L} & \Delta \\ \pm \Delta^* & -\mathcal{L}^* \end{pmatrix} \begin{pmatrix} u_q \\ v_q \end{pmatrix} = E_q \begin{pmatrix} u_q \\ v_q \end{pmatrix}$$

16 Byte × (2 × 97 × 97 × 161)² ~ 133 TB

Arnoldi / Lanczos iteration in Krylov subspace



Feasible future directions

✓ TDGPE + BdG in realistic **3D** systems

- collective modes of rotating BEC
- inclusion of dipolar interactions
- dynamics and collective excitations of
 F = 0, 1, 2, 3... spinor condensates, turbulence...
- BdG studies of s,p,d...-wave paired Fermi-systems
- superfluidity of graphene

in progress