1172-81-274 **Taras Lakoba*** (tlakoba@uvm.edu), University of Vermont, Dept. of Math & Stats, 82 University Place, Burlington, VT 05405. *Efficient solution of Hartree–Fock equations in a periodic external potential.*

Approximate yet fully quantum description of N impenetrable bosons in an external potential $V_{ext}(r)$ (e.g., helium atoms over a crystalline surface) leads to Hartree–Fock equations:

$$\big(-\nabla^2 + V_{ext}(r)\big)u_i(r) + \sum_{i\neq j}\langle u_j(r')|V_{bb}(r-r')|u_j(r')\rangle u_i(r) + \sum_{i\neq j}\langle u_j(r')|V_{bb}(r-r')|u_i(r')\rangle u_j(r) = \sum_j \mu_{ij}u_j(r), \quad (1)$$

where: u_i represents a one-particle wave function of boson i; ∇^2 is the Laplacian; $V_{bb}(r-r')$ is the interaction potential between bosons at locations r and r'; and μ_{ij} are Lagrange multipliers that make the solutions of (1) satisfy the orthonormality condition:

$$\langle u_i(r)|u_j(r)\rangle = \delta_{ij}. \quad (2)$$

Above, $\langle \ldots | \ldots \rangle$ denotes the standard inner product.

For an arbitrary V_{ext}, the cost of solving (1) increases as N^2, due to the second group of V_{bb}-terms and the μ_{ij}-terms. However, when V_{ext} is periodic, as typical in a crystal, one expects to be able to reduce this to one equation with $O(N)$ terms. In this talk we show how this can be implemented efficiently and the resulting equation can be solved iteratively. (Received August 30, 2021)