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The Dirac-Frenkel principle for reduced density matrices, and the Bogoliubov–de Gennes equations. (English summary)

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This work shows the existence and uniqueness of solutions for the non-linear, multibody, time-dependent Hartree-Fock equation. This is done using the Dirac-Frenkel principle (i.e., a variational principle with tangent projections) for two types of subspaces in Fock space: symmetrized (bosonic) and antisymmetrized (fermionic) states. Many aspects of these systems are covered in great detail, such as pairing densities applicable to Cooper pairs in the case of fermions, and the existence of a condensate in addition to quasifree states in the case of bosons.

The first part of the paper (sections 1–4) establishes the form of tangent projections for both types of statistics, and optimality is obtained precisely within the space of required solutions. The second part (section 5) uses Picard theory and careful norm estimates to prove convergence of nested integral series, and thus existence of solutions. This is indeed a very complete work and should be regarded as an achievement, given the non-linearity of the functionals containing the density and pairing functions.

Some remarks for the physicist: The problem of Coulomb interactions and the lack of convergence is circumvented by the authors with the introduction of an ad hoc Banach space, where fixed point theorems can be applied. The reader might be left wondering about the validity of proofs if a Yukawa (screening) regularization of Coulomb potentials is used instead; this is typically the case with misbehaved integrals in other contexts, such as scattering theory. In addition, the authors refer to their problem very early as bosonic or fermionic without the use of spin. While technically and mathematically correct, it is physically impossible to ignore spin for the effect of particle statistics. This is true even when the governing Hamiltonians do not contain spin interactions: textbook examples such as ortho- and para-helium states show the importance of spinors in the construction of solutions. Since Dirac himself ignored spin in early works about the Thomas atom, it is convenient to recall here the reference [P.A.M. Dirac, Math. Proc. Cambridge Philos. Soc. **26** (1930), no. 3, 376–385; JFM 56.0751.04].

For the mathematician, one should also mention that the Dirac-Frenkel principle was formally improved by A. D. McLachlan [Molecular Phys. **8** (1964), 39–44; MR0180123]. Important comments on this can be found in the Introduction of the following work [A. Raab, Chem. Phys. Lett. **319** (2000), no. 5-6, 674–678, doi:10.1016/S0009-2614(00)00200-1], including error estimates in further sections. *E. Sadurní*

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Note: This list reflects references listed in the original paper as accurately as possible with no attempt to correct errors.