RPA @ Paris 2010

Views and reviews of 50 years work

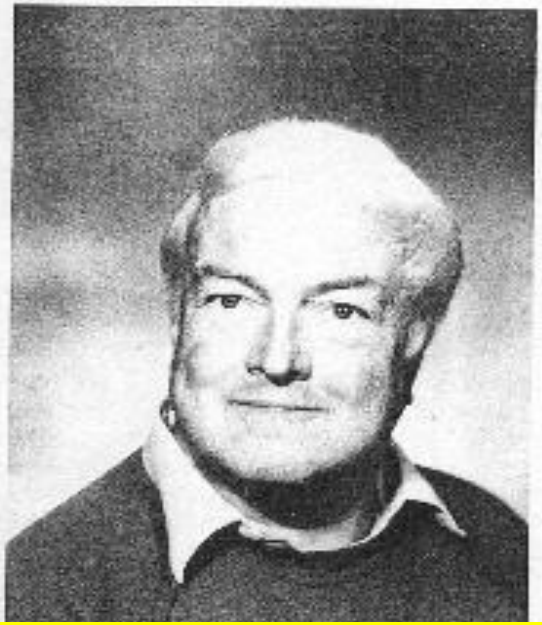
Jan Linderberg, Aarhus University

Mentors

PER-OLOV LÖWDIN

"Demanded" seminar on second quantization from a beginning student in September 1957

STIG OLOV LUNDQUIST



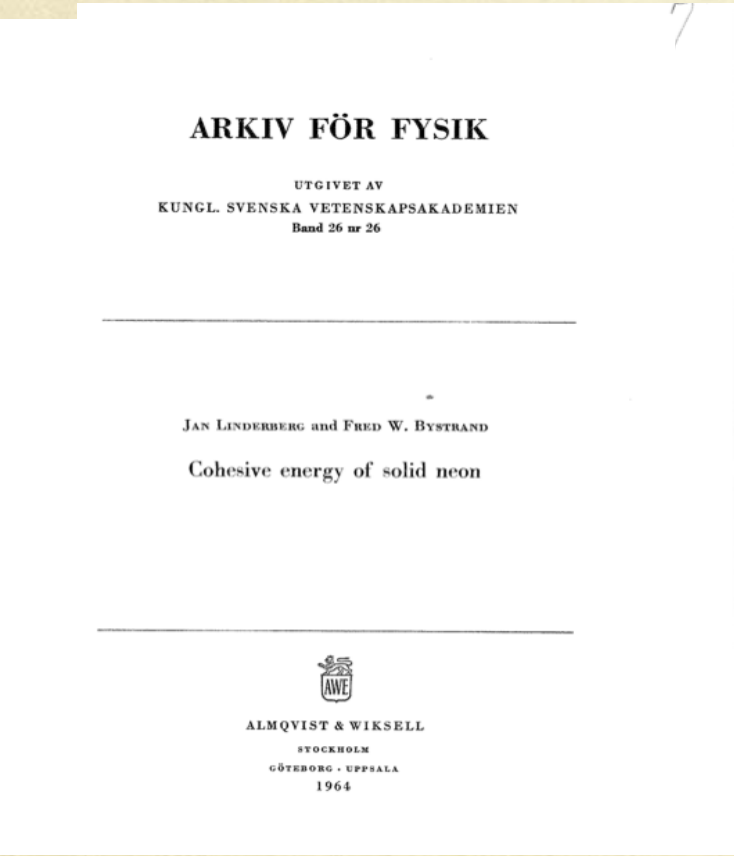
Introducedfieldmethods at the first Winter Institute at Gainesville December 1960

”Breakthru”

- Philippe Nozières and David Pines: *A dielectric formulation of the many body problem*, Nuovo Cimento **9**, 47 0 (1958)

- *On dispersion forces*, Physics Letters **1**, 272 (1962)

Cohesion in molecularXtals



ARKIV FÖR FYSIK

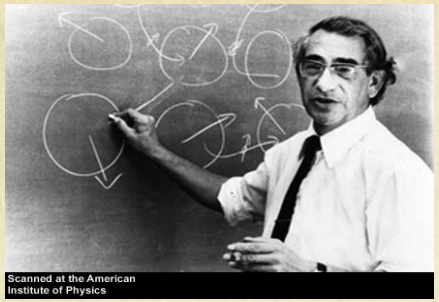
UTGIVET AV
KUNGL. SVENSKA VETENSKAPSAKADEMIEN
Band 26 nr 26

JAN LINDERBERG and FRED W. BYSTRAND

Cohesive energy of solid neon

ALMQVIST & WIKSELL
STOCKHOLM
GÖTEBORG · UPPSALA
1964

- Lindharddielectric approach
- Ehrenreich& Cohen:
  Timedependent HF
- Wannier: localization
- Cohen &Keffer: latticesums
- Dalgarno: polarizationorbital



Hubbard model

- J. Hubbard, *Electroncorrelations in narrowenergy bands*, Proc. Roy. Soc. **A276**, 238 (1963).

Improvedsingle-particlepropagators in the theory of conjugated systems, Proc. Roy. Soc. **A285,** 445 (1965)
Propagators for AlternantHydrocarbons, Phys. Rev. **139,** A1063 (1965)

Pariser-Parr-Poplemodel

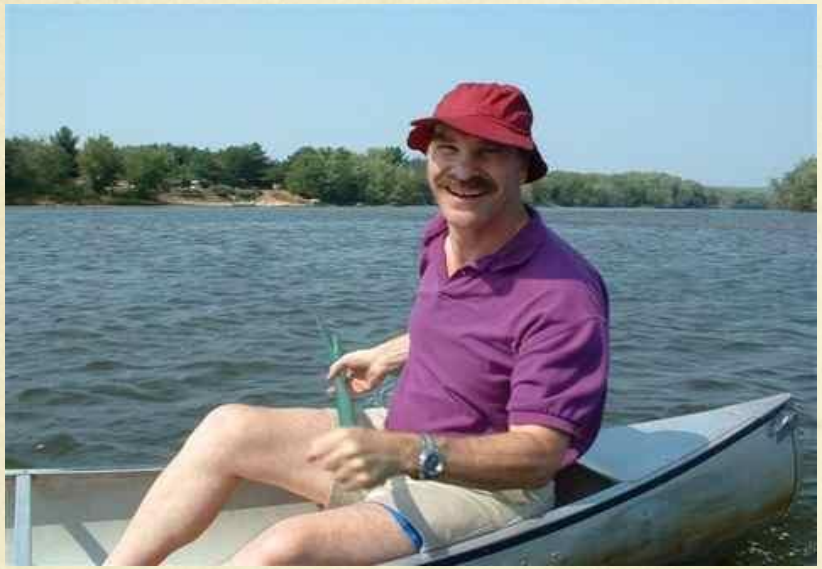
Poul Jørgensen

- Excitation energies
- Transition moments
- Eigenvaluealgorithm
- IJQC **4**, 587 (1970)

Lloyd Seamans

- Magneto-Optical Activity
- London, fielddependent, or bitals
- Mol. Phys. **24,**1393 (1972)

Formal stuff



- Mark Ratner
  - *Geometric approximation to two-particle Green function for Ethylene*, Chem. Phys. Lett. 7, 37 (1970)
  - *Self-consistent determination of the two-matrix by Coulson integration*

Self-ConsistentPolarizationPropagator Approximation as a ModifiedRandomPhaseMethod

- J. L., P. Jørgensen, J. Oddershede& M. Ratner
- *J. Chem. Phys.* **56**, 6213 (1972)
- Referencestaterenormalization
- General operator manifolds
- => SOPPA
- No formal groundstate!

On excitation energies

Statistics

Fermions

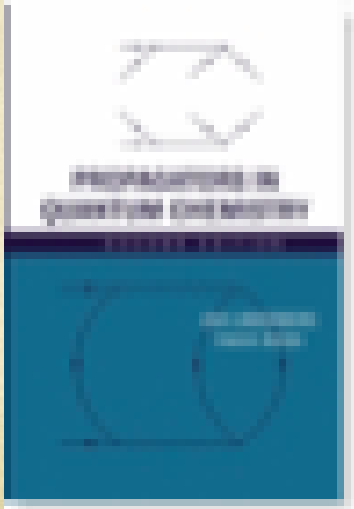
Bosons

Annihilators

State vectors and Propagators in Many-Electron Theory. A Unified Approach IJQC **12**, 161 (1977)
Characteristics of the Consistent Ground State of the Random Phase Approximation **15**, 343 (1979)

The antisymmetrizedgeminal power

Propagators in Quantum Chemistry, 2nd Edition



Propagators in Quantum Chemistry, 2nd Edition

Jan Linderberg, Yngve Öhrn

ISBN: 978-0-471-66257-0
Hardcover
267 pages
April 2004

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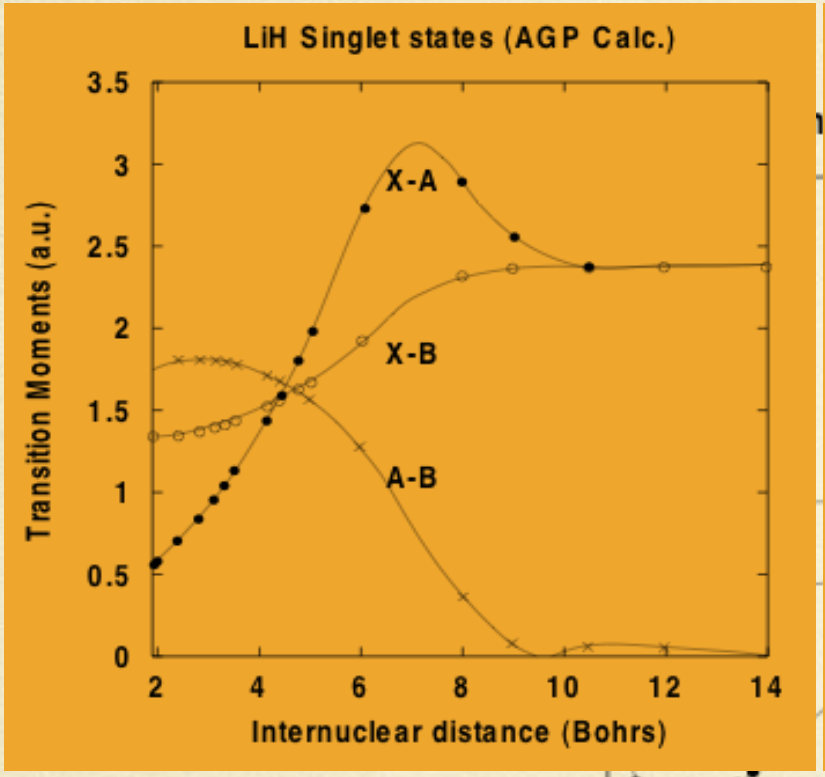
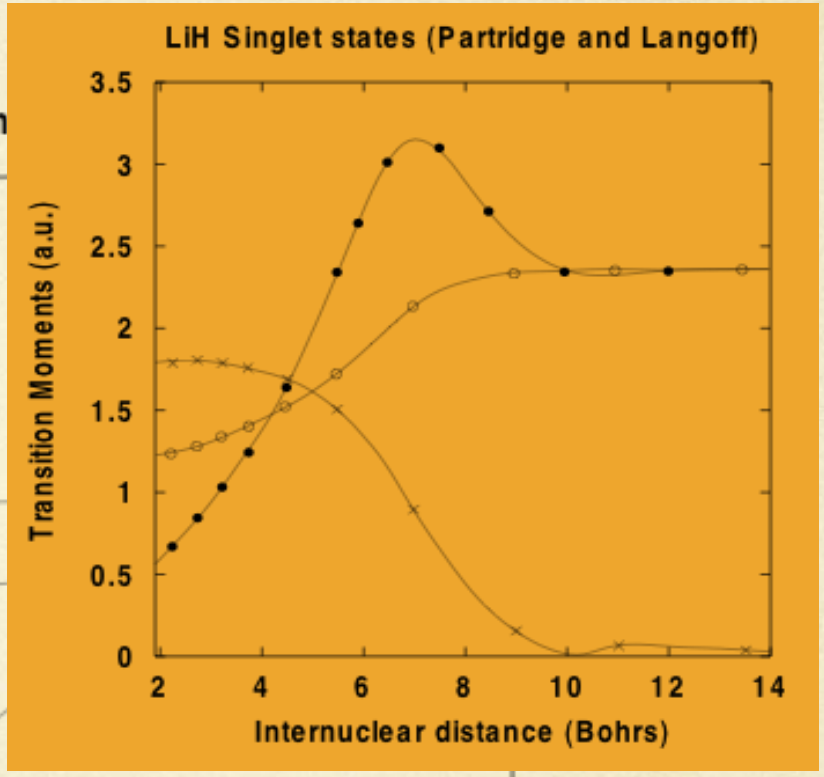
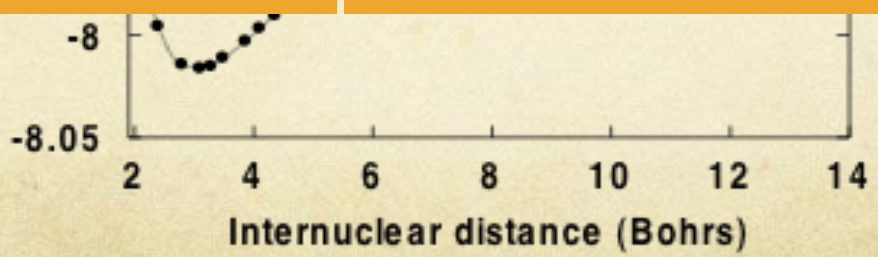
Example: LiH


LiH Singlet states (AGP Calc.)
Transition Moments (a.u.)
Internuclear distance (Bohrs)
X-A
X-B
A-B
0
0.5
1
1.5
2
2.5
3
3.5
2
4
6
8
10
12
14


LiH Singlet states (Partridge and Langoff)
Transition Moments (a.u.)
Internuclear distance (Bohrs)
0
0.5
1
1.5
2
2.5
3
3.5
2
4
6
8
10
12
14


-8
-8.05
2
4
6
8
10
12
14
Internuclear distance (Bohrs)

Example: Li_2

Table 5.2: $G(\nu)$ values for the first several vibrational states of the Li_2 ground state.

ν	KO[a]	AGP	EXP[b]
0	177.2	174.5	175.0
1	524.0	521.1	521.3
2	860.2	863.3	862.3
3	1189.3	1201.1	1198.0
4	1513.1	1534.0	1528.4
5	1832.4	1861.5	1853.5
6	2147.5	2183.6	2173.1
7	2458.4	2500.5	2487.2
8	2764.5	2811.7	2795.8
9	3065.7	3117.3	3098.7
10	3361.7	3417.3	3395.8

a.- KO refers to M. L. Olson and D. D. Konowalow, *Chem. Phys.* **22**, 129 (1977) and D. D. Konowalow and M. L. Olson, *J. Chem. Phys.* **71**, 450 (1979).

b.- EXP refers to M. Hessel and C. R. Vidal, *J. Chem. Phys.* **70**, 4439 (1979).

Continuum features

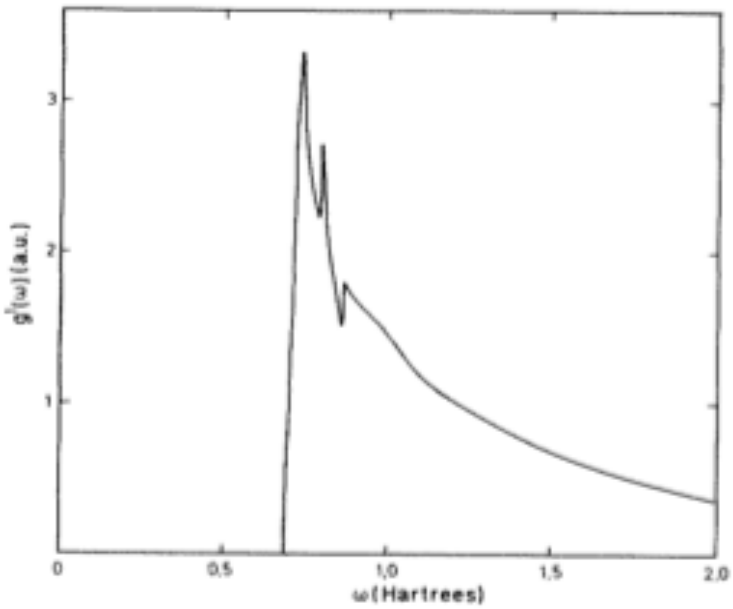


Figure 1. The differential oscillator strength distribution function $g^1(\omega)$ for helium, calculated by using the asymptotic approximation.

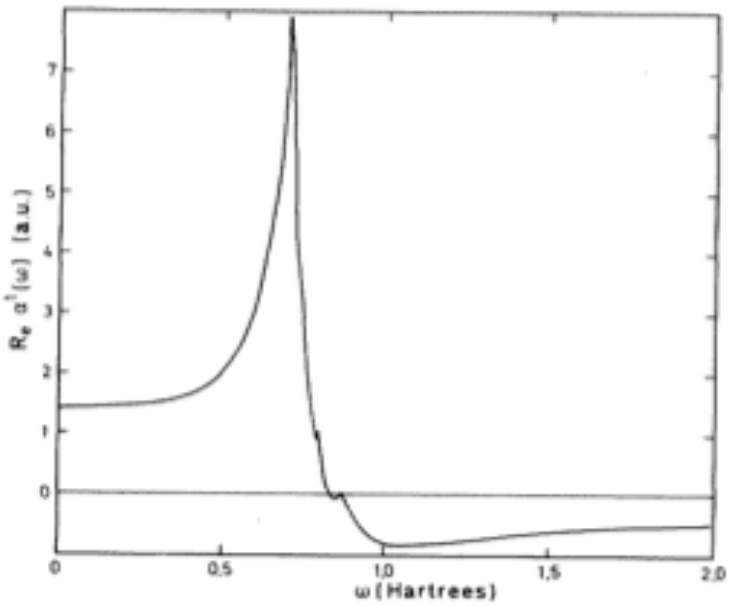


Figure 2. The dynamic dipole polarizability Re $\alpha^1(\omega)$ for helium, calculated by using the asymptotic approximation.

D. Prato & J.L. *Int. J. Quantum Chem.* **8**, 901 (1974).

Currenteffort

- Central fieldDiraceqn
- Static perturbations
- WKB electronpropagator
- Sphericaldecomposition
- Asymptoticevaluation of kernels

Thanks for the attention!

Artist: Bertil Blom