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Colloquium

The early scientific work (1976–2000) of E.K.U. Gross*

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Abstract. I review the scientific production of Eberhard K.U. Gross (Hardy Gross) in the first 25 years of his scientific career, from his study time at the Goethe University in Frankfurt am Main to the time he moved to the Free University of Berlin, as Full Professor. In between there was a fruitful period, in which he worked at the University of California, Santa Barbara, with Walter Kohn, the "father" of Density Functional Theory (DFT). DFT has been the permanent tool of Hardy Gross research. His main achievement in the considered period is the proof of an existence theorem for the Time-Dependent Density Functional (TDDFT) and the search for application schemes in atoms, molecules and solids, starting with linear response. He made notable contributions to the application of DFT and TDDFT to superconductors, in static and dynamic cases.

1 Introduction

I first met Eberhard K.U. Gross (Hardy Gross, born in Frankfurt in 1953) in September 1979 when I arrived to Frankfurt am Main, Germany, to start my PhD work under the supervision of Reiner Dreizler (born 1936), at the Goethe University (the place where Max Born taught in 1919–1921 and where the Stern–Gerlach experiment was performed in 1922). Hardy, a little older than me, was already a PhD student of the same professor of Theoretical Physics. We were therefore colleagues at the same group between September 1979 and December 1982. Hardy had already an aura of academic excellence, since it was known that he had won a first prize in a German Mathematics competition (1971) and that he got a fellowship from the Studienstiftung des Deutschen Volkes, a German Foundation which supports outstanding students. Indeed, he was the brightest student of the group working in the first floor of the Institute for Theoretical Physics, in the Robert Mayer Strasse, in the Senckenberg campus of the University (the big computer was in the basement and the well-stocked library was in the third floor). He was also a very kind person, always ready to help his colleagues. Hardy defended his PhD thesis (in the nomenclature used in Frankfurt, *Dr. Phil. Nat.*) in 1980. I keep a copy of his *Doktorarbeit* which was already centered on his favorite tool, Density Functional theory (DFT): *Der Dichtefunktional-Formalismus für Atome und quasimolekulare Zweizentren-Systeme und seine relativistische Erweiterung* ("Density-functional formalism for atoms and quasi-molecular two-center systems", #12 of Appendix; see Fig. 1). It was written at a time when there were no PCs and no word processors. From 1980 to 1984, he was Research Assistant at the Goethe University. In 1984, he spent three months at the University of Coimbra, Portugal, where I was Assistant Professor (I remember that he gave a very clear seminar on some conceptual problems of quantum mechanics), before spending 2 years at the University of California, Santa Barbara, supported by a NATO postdoc fellowship, to work with the already famous physicist Walter Kohn (1923–2016), the "father" of DFT and, strangely enough, Nobel laureate of Chemistry in 1998. In Santa Barbara, Hardy prepared his *Habilitation*, which he got in Frankfurt in 1985 (the title was *Dichtefunktionaletheory zeitabhängige Systeme*, "DFT of time-dependent systems", #26). From 1984 to 1990, he was Heisenberg Fellow at Santa Barbara, a prestigious scholarship of the Stifterverband für die Deutsche Wissenschaft (German Science Foundation), which allowed the researcher to choose any place to work during 5 years, to become in 1990 Fiebiger Professor at the University of Würzburg (the place where, in 1895, X-rays had been discovered by Wilhelm Roentgen, the first Physics Nobel prize winner; it is also the place of other Physics Nobel winners, such as Wilhelm Wien, Johannes Stark, and Klaus von Klitzing). In 2001, Hardy moved to the Free University of Berlin, a university founded after World War II and now high in the European rankings, leaving this place in 2009 to become Director of the Max Planck Institute of Microstructure Physics in Halle, founded in

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1992 as the first Max Planck Institute in the eastern part of Germany.

Here, I give an overview of the scientific career of Hardy Gross in the first 25 years, from 1976, the year of his first paper, co-authored with his *Doktorvater* Reiner Dreizler and published in *Phys. Lett. A*, which used the Thomas–Fermi potential, the crudest implementation of DFT, to 2000, his last full year in Würzburg before moving to Berlin. His most impressive scientific achievements in that period were as follows:

1. The paper in *Phys. Rev. Lett.* in 1984 containing the existence proof of a Time-Dependent Density Functional (TDDFT): E. Runge and E.K.U. Gross, "Density functional theory for time-dependent systems" (#22). That so-called Runge–Gross theorem is presently a textbook subject and there is even a Wikipedia entry on it. The paper has up to now more than 6000 citations in the Google Scholar, being his most cited work (it amounts to about one fifth of the total number of his citations).
2. The textbook written with his supervisor and published in 1990: R. M. Dreizler and E.K.U. Gross, *Density Functional Theory, an approach to the quantum many-body problem* (#38), now with ca. 4500 citations in the Google Scholar.

Paper #22 provided the conceptual basis for all work on TDDFT, an approach which was just a remote possibility at his PhD time in Frankfurt, when there were still discussions on the meaning of the existence theorem of Hohenberg and Kohn for the stationary case [1], but which is now mainstream. On the other hand, #38 is a reference work still in use today in spite of the numerous developments in DFT and the appearance of other reference books (e.g., Refs. [2,3]). Another important item of his bibliography was the co-edition, again with Dreizler, of the volume *Density Functional Theory*, Proceedings of the 1995 NATO Advanced Study Institute (ASI) held in August 16–27, 1993, in Il Ciocco, Tuscany, Italy (#50), a sequel of the famous ASI held in September 1983 in Alcabideche, Cascais, Portugal (which I attended as a recent PhD: I was given the job of escorting Kohn in Lisbon and I remember to attend a religious service with him at the Lisbon synagogue, where a security tried unsuccessfully to prevent our access since we were unknown there). The fact that Springer reprinted in 2013 the Il Ciocco volume indicates that it is still useful: in fact, it covers well the basic development of the DFT and applications in a variety of fields of physics (atomic, molecular, solid state physics, and nuclear physics) and chemistry.

2 Comments on Gross's publications

The list of E.K.U. Gross's works – including both papers and books – in the considered period is presented in the Appendix (the number of citations in *Google Scholar* is indicated at the end of each item, if bigger than ten). Table 1 summarizes his scientific production in the considered period, three sub-periods are distinguished: Frankfurt, Santa Barbara, and Würzburg.

Table 1. Bibliometric synopsis* of E.K.U. Gross's scientific production from 1976 to 2001 (Source: *Google Scholar*, May 27th 2018).

Year	# Papers	# Books	# Citations†
Frankfurt			
1976	1		
1977	0		
1978	2		
1979	6		124
1980	2	1	
1981	5		78
1982	2		47
1983	2		
Santa Barbara			
1984	2		6036
1985	2	1	921
1986	0	1	43
1987	1		78
1988	5		924
1989	2		40
Würzburg			
1990	2	1	1462
1991	1	1	11
1992	0		
1993	1		
1994	1		82
1995	7	1	501
1996	8		2499
1997	10		497
1998	4		408
1999	8		377
2000	6		657

*Total: 80 papers + 6 books = 86 works in 25 years. Annual average of works: 3.4 (peak in 1997, with 10 papers).
†Not considering papers with less than 10 citations.

2.1 Frankfurt period

In the Frankfurt period the total amounts to 21 works in 8 years with more than 249 citations. This is the formation period: Hardy was the author of 11 papers before the PhD defense, clearly above the average in those times.

The first paper (#1), written with his PhD adviser, a *Phys. Lett. A*, was on the use of Thomas–Fermi theory to describe quasi-molecular collisions. The theme of DFT kept being the subject of practically "all" his subsequent research. This paper brings together the main topics of Dreizler's theory group at the time: extended Thomas–Fermi approach to the stationary quantum many-body problem (extended meaning the inclusion of gradients of the density in the kinetic energy term as well as a local-density description of the exchange energy term) and the theoretical description of atomic and molecular collisions. Dreizler, obtained his PhD in Canberra (Australia) in 1964 and had been thereafter Assistant Professor at the Pennsylvania State University in Pittsburgh, USA, before becoming Professor of Theoretical Physics in Frankfurt in 1972. Starting from nuclear theory, he engaged in the late 1970s and the 1980s very actively in atomic and

molecular problems, both static or dynamic (although this essentially based on static snapshots).

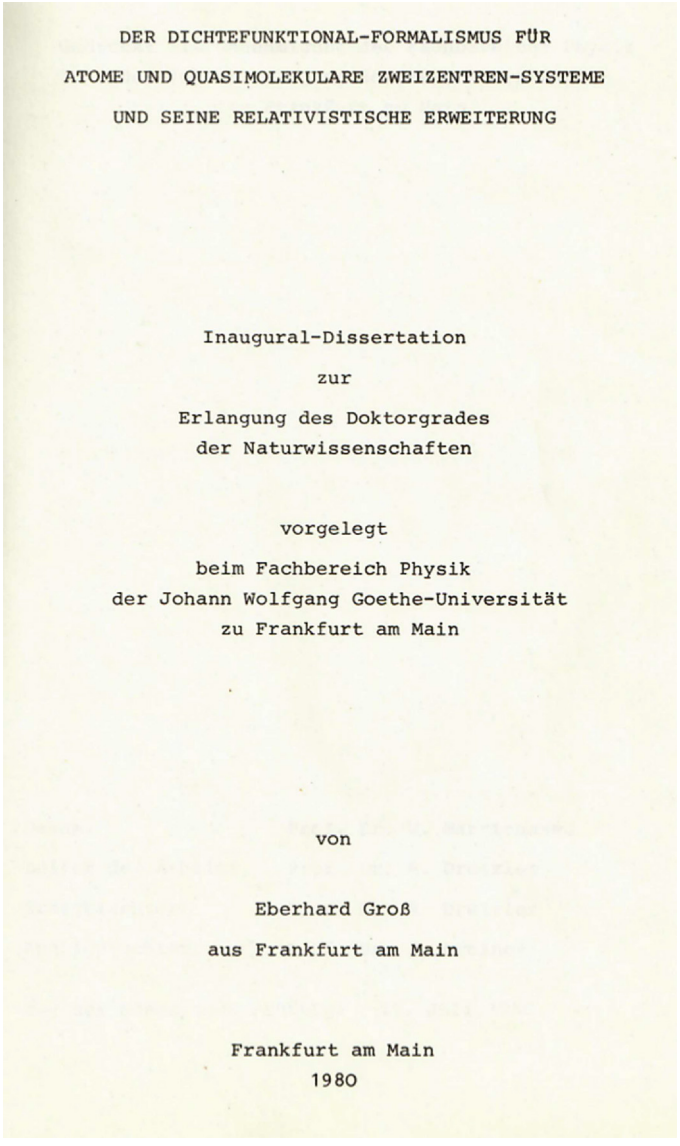
When I arrived in Frankfurt in September 1979, I got to know all of Hardy's co-authors in the Frankfurt period: Annie Toepfer, Hans-Juergen Luedde, Marko Horbatsch, Bernd Jacob, and Eberhard Engel were working in Extended Thomas–Fermi methods (from those only H.-J. Luedde and Eberhard Engel are now at the Goethe University). The only co-author not integrating this young group was Johann Rafelski (now at the University of Arizona in Tucson, USA, #5), then an associate to Walter Greiner (1935–2016), who was Director of the Institute for Theoretical Physics and head of a bigger group doing nuclear, particle theory, and electrodynamics of strong fields. At the time a dream in Frankfurt was the discovery of superheavy elements, which was pursued at the nearby Gesellsachft für Schwerionen Forschung GSI, in Darmstadt, but did not come to fruition. I was the last student of Dreizler in nuclear theory (I used in my PhD the Generator Coordinate Method to describe the inertia parameter in nuclear fission), so that I was not involved in the work on atomic or molecular systems. Only in 1991, when nuclear physics was declining after the Chernobyl disaster, I moved to DFT, working on atomic clusters, surfaces, and crystals with John Perdew (born in 1943), then professor at the Tulane University, New Orleans, USA, now at the Temple University, near Pittsburgh, Pennsylvania. The most quoted paper of Hardy in 1979 (#8) was on a numerical solution of the Extended Thomas-Fermi equation for atomic and molecular systems,

1980 is the year of Hardy's PhD (#12, see Fig. 1), where he presented a careful study of the density gradient terms which should be added in a systematic way to the Thomas–Fermi treatment of the kinetic energy to improve accuracy, both non-relativistic and relativistic. In the next year, the most cited paper, having Hardy and his supervisor as single authors (#15), was on the treatment of the exchange energy (Dirac term). Semiclassical treatments of this type were also popular in nuclear physics, as shown by the title of a meeting in Grenoble which I attended (#16 and #17). Although this interdisciplinary dialogue was very fruitful, it turned out that DFT gained more momentum in its application to electronic systems where, in comparison with nuclear physics, the interaction is exactly known.

Hardy's most cited paper in 1982 (#19) continues the semiclassical handling of atomic systems of the Frankfurt group. Dreizler had an Australian PhD, but, since an ex-collaborator claimed that he was not entitled to use the German doctor title, he just presented a doctoral dissertation in 1981 [4] on the relativistic version of Extended Thomas Fermi theory. Due to this rather peculiar circumstance, Hardy should have been one of the few students to have defended his PhD thesis before his supervisor did the same at the same university. Hardy wrote jointly with Dreizler 21 papers from 1976 to 1985.

2.2 Santa Barbara period

The Santa Barbara post-doc period (see Fig. 2) encompasses 14 works in 6 years with more than 8042 citations.


DER DICHTEFUNKTIONAL-FORMALISMUS FÜR

ATOME UND QUASIMOLEKULARE ZWEIZENTREN-SYSTEME

UND SEINE RELATIVISTISCHE ERWEITERUNG

Inaugural-Dissertation

zur

Erlangung des Doktorgrades

der Naturwissenschaften

vorgelegt

beim Fachbereich Physik

der Johann Wolfgang Goethe-Universität

zu Frankfurt am Main

von

Eberhard Groß

aus Frankfurt am Main

Frankfurt am Main

1980

Fig. 1. Front page of Hardy's PhD thesis.

This time includes Hardy's collaboration with Kohn. They wrote together 9 papers from 1985 to 1990.

1984 is the year when the most cited piece of work of Hardy (#22) came out, although it had been prepared before. It was written together with a younger colleague with whom he would write a textbook on many-body theory, with German and English editions (#27 and #40). Erich Runge (born in 1959), as Hardy, a laureate with a national mathematics prize as high-school student, finished his *Diplom* with Dreizler in Frankfurt in 1984 and did his PhD in Stuttgart in 1990. Since 2004, he is Full Professor and since 2011 Director of the Institute of Physics of the Technical Institute Ilmenau, Germany. According to the Runge–Gross theorem, there is a one-to-one mapping between the potential in which a quantum many-body system develops, starting from a given instant, and the corresponding density. The proof lies on the Taylor expansion of the external potential (e.g., an electric field) about the initial time. There were later extensions

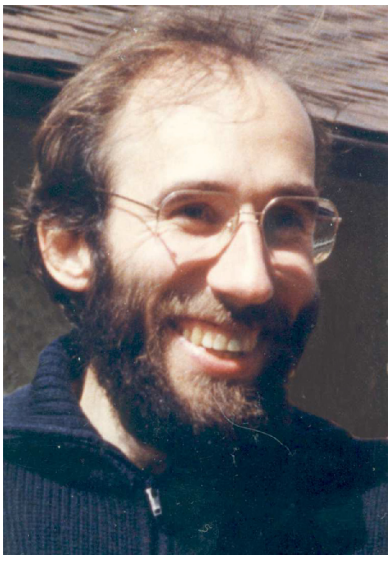


Fig. 2. Hardy Gross in Santa Barbara.

to statistical situations, to multi-component systems (i.e., systems with several densities), to magnetic systems which require the vector potential, and to superconductivity.

1985 is marked by the publication of the proceedings of the influential Alcabideche conference (#24), held close to Lisbon, Portugal, which were edited by Reiner Dreizler and João da Providência (born in 1933), professor of Theoretical Physics at the University of Coimbra who had been in the 1960s PhD student of Sir Rudolf Peierls (1907–1995), and also by Hardy's *Habilitation* (#25). It is also marked by Gross and Kohn's first common work (#25), on a particular approximation to the TD problem, namely, the local-density approximation (LDA) to the frequency-dependent exchange-correlation potential. In fact, both met for the first time in Portugal [5] in the Alcabideche conference and Kohn became then enthusiastic about the possibility of TD developments of his theory.

1986 had been a rare scarce year in Hardy's production with only a brief paper, on the Gross–Kohn TDDFT scheme, but in the next year he wrote four papers with Kohn, all of them well cited, handling temperature-dependent DFT (#29 and #30) and its application to superconductivity (#32), a phenomenon which was going to be a challenge to Hardy and his collaborators. One of them was a Brazilian physicist, Luís N. Oliveira, from the University of São Carlos, São Paulo (they wrote nine papers together, e.g., #29). In 1989, Hardy and Kohn continued their work on superconductivity.

2.3 Würzburg period

In the Würzburg period (see Fig. 3), there was a total of 51 works in 11 years with more than 6494 citations. This is Hardy's first professorship period in Germany, when he created his own group. His fame was progressively rising with the accumulation of works and citations.

1990 is the year of a review of TDDFT in a chemistry journal (#36). It is clear that TDDFT was attracting the interest of more people, in Physics as well as in Chemistry, since stationary DFT was already becoming current in Chemistry, after his remarkable success in Condensed Matter Physics using the LDA. Various phenomenological approaches were proposed by chemists, while physicists were trying to find first-principles schemes, in the framework of the so-called Generalized Gradient Approximations (GGA), which replaced Extended Thomas–Fermi. The classic Springer textbook by Dreizler and Gross (#38) appeared in that year: it would be cited by Kohn in his Nobel lecture.

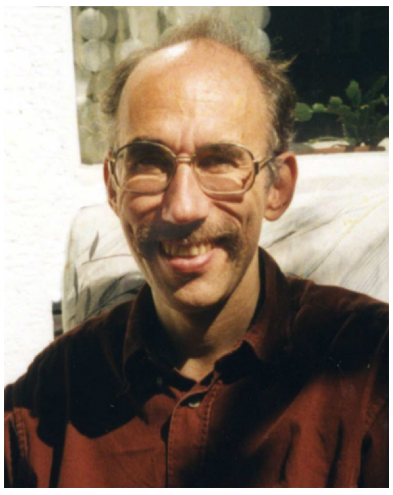


Fig. 3. Hardy Gross in 1997.

In 1991, the Gross and Runge German textbook on many-body theory (#27) was translated into English (#40), from the second edition, with the addition of a third author and a new chapter on Fermi liquid theory

In 1994, paper #42 was the first application of TDDFT to superconductivity: analogues of Hohenberg–Kohn and Kohn–Sham theorems were presented. More students were then clustering around Hardy, who changed from being first author to be last one in most papers, reflecting his progressive seniority. The most cited paper of 1995 is a *Phys. Rev. Lett.* on an optimized TD potential (#43). Hardy was co-editor in this year of the Proceedings of the NATO ASI held in Il Ciocco, Italy, in 1993, on DFT (#50), which contains reviews with Hardy as first author on superconductivity with DFT and TDDFT, as well as reviews of DFT by Kohn and Perdew.

There is in this period a clear pattern in Hardys's publications: they were either reviews, giving an overview of some aspect of DFT, or letters in top journals, providing timely advances. In 1996 his most cited work was a *Phys. Rev. Lett.* (#57) on how to calculate atomic and molecular excitation energies from TDDFT, followed by another review on TDDF (#54), in a chemistry journal. The interest of chemists by DFT was clearly increasing at that time. In 1997 the most cited work of Hardy was another *Phys. Rev. Lett.* on TDDFT (#65), now, going beyond linear response by incorporating memory effects in the exchange-correlation potential.

In 1998, his most cited work was another review of TDDFT, in the 500th volume of the series "Springer Lecture Notes in Physics" (#69). This year was very important to the DFT community due to the award of

the Chemistry Nobel prize to Kohn (in the company of John Pople 1925–2004). This was the "official" recognition of the usefulness of DFT in Chemistry, which was already clear in Physics.

In 1999 the most cited work of Hardy was a trial of DFT to describe the van der Waals chemical binding (#73), a challenge which persists today. In #79, Miguel Marques, a Portuguese PhD student of Hardy coming from the University of Coimbra, appears for the first time in Hardy's publication list. He completed his PhD on superconductivity and wrote with him 24 other papers. He is now at the University of Halle, Germany. Another frequent co-author of Hardy at this time was K. Capelle, with 11 joint publications.

Finally, in 2000, the most cited work was a *Phys. Rev. Lett.* containing a TDDFT description of helium ionization by an ultra-short laser pulse (#86). Another paper with a reasonable number of citations is co-authored with John Perdew (#83), one of the big names of DFT (Hardy wrote two papers with him).

3 Conclusions

Here, I sketched the first 25 years of the scientific life of E.K.U. Gross (Hardy Gross), just the first part of a career which continued in a very dynamic way until the present day. In 2017, Hardy became Professor of Chemistry at the Hebrew University of Jerusalem, the place which keeps the heritage of Albert Einstein.

Hardy revealed his unusual talent for Theoretical Physics already at the very beginning of his academic studies. He is the most successful disciple of Reiner Dreizler, the German great promoter of DFT and its application to atomic and molecular systems (we may speak of a Frankfurt school). Hardy, besides being the author with his supervisor of an early textbook in the subject, presented in 1984 the first proof of existence of TDDFT, opening a field which is nowadays very florescent (see e.g., Refs. [6,7]). He also made relevant contributions to the ab-initio description of superconductivity

Since the Summer School of 1983 held in Alcabideche, Portugal is related to the DFT history. Twenty years later there was another School on DFT, organized in Caramulo, Central Portugal, by the Center for Computational Physics (nowadays Center for Physics) of the University of Coimbra. In the School official dinner, the ex-students and friends of Prof. Dreizler offered him, since his retirement was approaching, an original edition of an eighteenth century book by Leonhard Euler on variational principles. The choice was justified because DFT adopts a variational approach to solve the Schrödinger equation for many-body systems. But he may also be justified because Euler is the most prolific mathematician of all time: he wrote hundreds of articles and books. With the due differences, Dreizler has also a very extensive scientific production in papers and books in different fields of Physics: 326 papers are available at Research Gate and 21 books are available at Amazon; he is still publishing Physics textbooks. Now the time for Hardy's academic retirement has arrived, a circumstance which does not mean scientific retirement. Like his mentor, he continues to be extremely active: he counts by now more than 270 articles (including book chapters) and 8 books, with a total of more than 30,000 citations. If his work can be summarized in a single number, we may use the *Google Scholar* h-index of 67, that is, 67 works have received at least 67 citations each. Since he continues to be extremely active, much more is still expected from him.

I am indebted to Ana Serôdio, the librarian who reviewed the list of publications in the Appendix, and to Angelica Zacarias for providing the photographs of Hardy.

Appendix: List of E.K.U. Gross's works (1976–2000)

Frankfurt period

1976

1. E.K.U. Gross and R.M. Dreizler, "Thomas-Fermi potentials for quasimolecular collision processes", *Phys. Lett. A* **57**, 131–134.

1978

2. B. Jacob, E.K.U. Gross, and R.M. Dreizler, "Solution of the Thomas-Fermi equation for triatomic systems", *J. Phys. B At. Mol. Phys.* **11**, 3795–3802.
3. E.K.U. Gross, M. Horbatsch, and R.M. Dreizler, "Multi-state impact parameter approximation for many-particle excitations in atomic collisions, total cross-sections for Na-Ne and N-Ne", *Z. Phys. A* **285**, 353–356.

1979

4. R.M. Dreizler, E.K.U. Gross, and A. Toepfer, "Extended Thomas-Fermi approach to diatomic systems", *Phys. Lett. A* **71**, 49–53 (14 cits).
5. E.K.U. Gross and J. Rafelski, "Electromagnetic potential in Thomas-Fermi-Dirac atoms", *Phys. Rev. A* **20**, 44–45 (10 cits).
6. E.K.U. Gross, A. Toepfer, B. Jacob, and R.M. Dreizler, "Extended Thomas-Fermi approach to screening effects in atoms and quasimolecular systems", in I. Iori, ed., *Proc. of the XVII International Winter Meeting on Nuclear Physics in Bormio*, (Milano, Italy), pp. 68–94.
7. H.J. Luedde, M. Horbatsch, E.K.U. Gross, and R.M. Dreizler, "Time-dependent description of atomic scattering problems", in I. Iori, ed., *Proc. of the XVII International Winter Meeting on Nuclear Physics in Bormio*, (Milano, Italy), pp. 120–136.
8. E.K.U. Gross and R.M. Dreizler, "Thomas-Fermi approach to diatomic systems I. Solution of the Thomas-Fermi and Thomas-Fermi-Dirac-Weizsaecker equations", *Phys. Rev. A* **20**, 1798–1807 (87 cits).
9. A. Toepfer, E.K.U. Gross, and R.M. Dreizler, "Thomas-Fermi approach to diatomic systems. II. Calculation of correlation diagrams and total molecular energies", *Phys. Rev. A* **20**, 1808–1815 (27 cits).

1980

10. R.M. Dreizler, E.K.U. Gross, M. Horbatsch, B. Jacob, H.J. Luedde, and A. Toepfer, "Towards a description of relativistic screening effects in diatomic systems", in *Procs. of the XVIII International Winter Meeting on Nuclear Physics in Bormio in 1980, Ricerca Scientifica ed Educazione Permanente*, sup. **13** (Milano, Italy), pp. 764–797.
11. A. Toepfer, E.K.U. Gross, and R.M. Dreizler, "Thomas-Fermi approach to diatomic quasimolecules: Correlation diagrams for neutral, heteronuclear systems", *Z. Phys. A* **298**, 167–171.
12. E.K.U. Gross, *Der Dichtefunktional-Formalismus für Atome und quasimolekulare Zweizentren-Systeme und seine relativistische Erweiterung*, *Dr. Rer. Nat.* dissertation, Goethe University, Frankfurt am Main, 146 pp.

1981

13. E.K.U. Gross and R.M. Dreizler, "Relativistic gradient expansion of the kinetic energy density", *Phys. Lett. A* **81**, 447–450.
14. B. Jacob, R.M. Dreizler, and E.K.U. Gross, "Solution of the extended Thomas-Fermi model for triatomic molecules", *J. Phys. B: At., Mol. Opt. Phys.* **14**, 2753–2759.
15. E.K.U. Gross and R.M. Dreizler, "Gradient expansion of the Coulomb exchange energy", *Z. Phys. A* **302**, 103–106 (78 cits).
16. R.M. Dreizler, M. Horbatsch, H.J. Luedde, E.K.U. Gross, and A. Henne, "Time-dependent description of atomic collisions", in P. Quentin and P. Schuck, eds., *Semiclassical methods in Nuclear Physics*, (Institut Laue-Langevin, 18, Grenoble, March 20, 1981), pp. 1–10.
17. R.M. Dreizler, E.K.U. Gross, B. Jacob, A. Toepfer, and W. Stich, "Density-functional approach to many-body Coulomb systems", in P. Quentin and P. Schuck, eds., *Semiclassical Methods in Nuclear Physics*, (Institute Laue Langevin 18, Grenoble, March 20, 1981), pp. 11–14.

1982

18. E.K.U. Gross and E. Runge, "Functionals of fractional form in variational scattering theory", *Phys. Rev. A* **26**, 3004–3007 (1982).
19. W. Stich, E.K.U. Gross, P. Malzacher, and R.M. Dreizler, "Accurate solution of the Thomas-Fermi-Dirac-Weizsaecker variational equations for the case of neutral atoms and positive ions", *Z. Phys. A* **309**, 5–11 (47 cits).

1983

20. R.M. Dreizler and E.K.U. Gross, "Density functional approach to the relativistic many-body problems", in W. Greiner, ed., *Quantum Electrodynamics of Strong Fields*, Proc. NATO ASI held in Lahnstein on the Rhein, June 15–26, 1981 (Plenum Press, New York), pp. 383–412.
21. E.K.U. Gross, A. Toepfer, B. Jacob, M. Horbatsch, H.J. Luedde, and R.M. Dreizler, "Density functional approach to molecular structure and atomic scattering", in J. Berkowitz and K.O. Groeneveld, eds., *Molecular Ions, Geometric and Electronic Structures*, NATO ASI held in Koos, Greece, September 30–October 10, 1980 (Plenum Press, New York), pp. 419–422.

Santa Barbara period

1984

22. E. Runge and E.K.U. Gross, "Density functional theory for time-dependent systems", *Phys. Rev. Lett.* **52**, 997–1000 (6036 cits).
23. E.K.U. Gross and R.M. Dreizler, "Relativistic density functional theory", in. J.P. Dahl and J. Avery, eds., *Local Density Approximations in Quantum Chemistry and Solid State Physics* (Plenum Press, New York), pp. 353–379.

1985

24. E.K.U. Gross and R.M. Dreizler, "Density functional approach to time-dependent and to relativistic systems", in R.M. Dreizler and J. da Providência, eds., *Density Functional Methods in Physics*, Proc. of the NATO ASI held September 5–16, 1983, in Alcabideche, Portugal (Plenum Press, New York), pp. 81–140.
25. E.K.U. Gross and W. Kohn, "Local density functional theory of frequency-dependent linear response", *Phys. Rev. Lett.* **55**, 2850–2852 (921 cits).
26. E. Gross, *Dichtefunktionaltheorie zeithabhaengige Systeme*, University Goethe, Frankfurt am Main, *Habilitation schrift*, 79 pp.

1986

27. E.K.U. Gross und E. Runge, *Vielteilchentheorie*, (Teubner, Stuttgart), 399 pages (43 cits).

1987

28. N. Iwamoto and E.K.U. Gross, "Correlation effects on the third frequency moment sum rule of electron liquid", *Phys. Rev. B* **35**, 3003–3004 (78 cits).

1988

29. E.K.U. Gross, L.N. Oliveira, and W. Kohn, "Rayleigh-Ritz variational principle for ensembles of fractionally occupied states", *Phys. Rev. A* **37**, 2805–2808 (242 cits).
30. E.K.U. Gross, L.N. Oliveira, and W. Kohn, "Density functional theory for ensembles of fractionally occupied states. I. Basic formalism", *Phys. Rev. A* **37**, 2809–2820 (257 cits).
31. L.N. Oliveira, E.K.U. Gross, and W. Kohn, "Density functional theory for ensembles of fractionally occupied states, II. Application to the He atom", *Phys. Rev. A* **37**, 2821–2833 (147 cits).
32. L.N. Oliveira, E.K.U. Gross, and W. Kohn, "Density functional theory for superconductors", *Phys. Rev. Lett.* **60**, 2430–2433 (266 cits).

33. E.K.U. Gross, D. Mearns, and L.N. Oliveira, "Zeros of the frequency-dependent linear density response", *Phys. Rev. Lett.* **61**, 1518–1519 (12 cits).

1989

34. W. Kohn, E.K.U. Gross, and L.N. Oliveira, "Density functional theory for superconductors", *Int. J. Quant. Chem. Symp.* **23**, 611–615.
35. E.K.U. Gross, L.N. Oliveira, and W. Kohn, "Orbital magnetism in the density functional theory of superconductors", *J. Phys. (Paris)* **50**, 2601–2612 (40 cits).

Würzburg period

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