Volume 1, Issue 2, July 2011

# JUNQ

## Journal of Unsolved Questions

# Honesty in Science

## Highlights

### Working as an Ombudsman of Science
with Prof. Dr. Siegfried Hunklinger

### The Schön scandal
Interview with Prof. Dr. Gerhard Fröhlich

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# Preface

## Editorial Note

*Dear Reader,*

it is my great pleasure to present to you this second issue of JUnQ, the Journal of Unsolved Questions. To me this is a solemn occasion and I invite you to stop for a moment. Let us reflect on the still short history of the journal. The first issue was published half a year ago and it contained three clear objectives, outlined in our mission statement: Offering scientists the possibility to publish their negative and null-results in an article and thereby helping to overcome biases and fraud in research, publishing essays on open questions as science is driven by questions rather than answers, and, finally, establishing a platform for reflecting on the mechanisms governing the daily routine of science. The successful publication of the first issue encouraged us to further pursue the project, but although being convinced of the idea of JUnQ, we could not know if scientists appreciated it and availed themselves of the possibility to contribute. So, the crucial question was: Would JUnQ remain just an unconventional but transient idea or would it turn into a widely recognized journal, to which scientists would be eager to submit their manuscripts? There was, and is, no obvious answer, but I would like to outline my personal answer in this editorial note.

In the first issue, we promised our readers a biyearly release of JUnQ and with this second issue we are true to our word. We obtained an ISSN number and applied for Thomson Reuters' Web of Science. But as promising as this formal progress looks, we need to remind ourselves that a scientific journal is only as good as the contributions it contains. So, let us take inventory. The first issue contained two articles on null-result research and four open questions and with this second issue, we present another article and four open questions. It is the authors of all these contributions, to whom I feel first and foremost obliged. Only their audacity to submit an article to JunQ enabled us to publish this second issue. Why do I emphasize this so much? It always requires some courage to publish scientific results in a new and not yet established journal, but JUnQ is a journal that publishes negative results and this makes it special among the scientific journals in the world. This special character carries consequences that could keep people from submitting their article. There is hardly an argument over the importance of negative results, but it is controversial, if and in which form they should be made public. Null results are always unexpected results and yet, although most scientists freely admit that they are a commonplace occurrence even in their own research projects, nobody likes to admit that a project remained unsuccessful.

The reasons for this behavior are numerous, but let us exemplify a few of them by considering a complicated synthesis in organic chemistry. This typically involves a group of several dozen people, all working on their own piece of the problem, but united in one goal: Finding the first practicable way to synthesize a highly complicated molecule. Now, let us assume that a single step in a reaction cascade does not work out and thereby hinders completion of the whole project. At the same time, a rival group aims at the same target molecule and may be just one step away from the final breakthrough. In this situation, the group's first priority is to find an alternative route to the target molecule, it is not to investigate why the crucial step failed and account for the unsuccessful attempt by writing an article for publication to be shared with the scientific community. You may consider this as an issue specific to organic synthesis, but it is, in a metaphorical sense, common to all science: Scientists want to invest their energy where it matters and the benefit of sharing knowledge about a new unsuccessful attempt is sometimes not obvious. Getting back to organic synthesis, I would like to illustrate two further problems inherent to the publication of negative results: It is often an arduous and cumbersome task to ascertain that the negative outcome of a reaction is not due to contaminations, inadequate reaction control, or comparable trivial reasons. This phenomenon also corresponds to a fact common to all science: You can never be sure that the reason for failure is non-trivial and you may fear that another scientist reading about your failure would promptly realize, where you made your mistake. In consequence, your fear of being regarded as inept and foolish keeps you from publishing your negative result. The third reason that hinders negative results from being published is as follows, exemplified by organic synthesis: Once it is clear that a certain synthesis route is not passable, a scientific group wants to keep this knowledge private, as the considerable efforts on which it is based are often not acknowledged, while at the same time they could benefit rival groups and enable them to gain the glory.

At this point, I could conclude by simply stating that the nature of negative results inevitably prevents them from being published. That would be a convenient answer to the introductory question. However, it would mean that scientists are no longer willing to cope with their problems, that they only aim at quick, but ephemeral success, and are mainly driven by the desire to outpace each other. My fellow readers, I utterly reject this view. I am convinced that scientists feel foremost obliged to those values that transcend personal success and evanescent fame: sincerity, honesty, progress, and scientific freedom. There will be a simple answer to the introductory question if you and I have the courage to share not only our answers, but our questions and our incomprehension as well. So, will JUnQ survive? My answer is an emphatic and unequivocal "yes"! JUnQ will survive since publishing negative results and open questions will benefit all of us. Selective publication of data distorts scientific methods, creates various biases, and keeps us from maintaining full productivity. We need to realize that negative results are not always liabilities, they may turn into assets. A finding that seems incomprehensible now may be comprehended ten years later and it is only today's questions that make up tomorrow's explanations.

I would like to complete this reflection on the future of JUnQ with a special note to our readers from the social sciences and humanities: you may consider the upheavels that led to the foundation of JUnQ as specific to natural science, but they are not. The idea of JunQ transcends sectional boundaries and the fact that the two issues published so far mainly focus on natural science is not intended, but rather due to the framework, from which JUnQ originated. I invite you all to contribute and I hope that you have the audacity to submit a manuscript that does not fit in the formats provided at the moment. Still experimental, JUnQ will spare no effort to find novel formats that suit your needs.

True to our mission statement, JUnQ intends to be more than a scientific journal, but it aims at providing a platform to reflect on the principles of science. This second issue you are reading is dedicated to "Honesty in Science". When we initiated the lecture series "Publish or Perish" at the beginning of this year, the announced title of Professor Hunklinger's talk "Honesty in Science" was just one out of several. But the following political events in Germany showed that this title was ahead of its time. Pushed by plagiarism allegations against the German minister of defense related to his doctoral thesis, which finally forced him to resign, a vital public debate on honesty in science emerged and drew the German media's attention to JUnQ. This special issue is our contribution to that debate. It contains an interview with ombudsman for science Siegfried Hunklinger, a review on Eugenie Reichs book "Plastic Fantastic", which deals with the scandal around physicist Jan-Hendrik Schön, and an interview with Austrian philosopher of science Gerhard Fröhlich on the Schön scandal.

"Honesty in Science" is a grand word with many facets that is too important to be left only to philosophers. We cannot avoid it as we encounter it everyday. Who does not remember the desire to exclude that single set of data that distorted all results? Who never felt the urge to reuse those elegant formulations read in another publication? Who thinks that he acknowledged all supporters in his publications? Scientific misconduct occurs in numerous ways and to different degrees of severity. Another essay would be needed to account for the different faces of misconduct in natural science, social science, and the humanities, but such a reflection is beyond this note. However, I would like to comment on a different issue. A frequently proposed solution to cope with scientific misconduct consists in introducing yet another regulation program or ethics committee. Meanwhile, a growing mistrust against each other drives the scientific community to curtail its freedom. Science is now more regulated than 50 years ago, but did this regulation help to reduce fraud and misconduct? There is no obvious answer, however, we should remember roman historian Tacitus' statement: The more corrupt the state, the more laws. As ombudsman Professor Hunklinger points out, we will never be able to completely avoid it. Let there be no misunderstanding. It is not my intention to do away with all those regulations, but rather to remind you that we should not shift the problem to some institution and forget about it. Instead, it is our responsibility to live up to those values of which I spoke earlier. No organization and no ethics committee will prevent us from fraud and misconduct as long as we do not feel obliged to hold to those values. I hope that this special issue of JUnQ and the contributions therein will suit that purpose.

The business of JUnQ goes forward. We aim at presenting the next issue on January 1st, 2012 and we are convinced that it will contain various contributions not only from natural science, but also from the social sciences and humanities. We will continue our lecture series at the University of Mainz with a different focus and we hope that a steadily growing number of people join in our crusade.

Concluding this editorial note, we would like to express our gratitude to all supporters of JUnQ. In particular, we thank all authors once more for their courage to contribute as well as all speakers and debaters for participating in the lecture series "Publish or Perish". Furthermore, we acknowledge the interest of various newspapers, broadcasting companies, and journalists. Their stories about JUnQ and the opportunity to have interviews were crucial to spread the knowledge of JUnQ. We feel also indebted to the Stifterverband für die Deutsche Wissenschaft for having awarded JUnQ "Hochschulperle des Monats" in April 2011. Finally, we would like to thank the graduate school Materials Science in Mainz and the Johannes Gutenberg-Universität Mainz, whose generous support helped us in all fields of action.

We are looking forward to receiving your manuscript for publication!

*Thomas Jagau on behalf of the editorial board*

## Quotes on JUnQ from the Press

*The Journal of Unsolved Questions has been awarded the "University Pearl" for April 2011 by the Stifterverband für die deutsche Wissenschaft.*

Doktoranden der Graduiertenschule "Materials Science" an der Johannes Gutenberg Universität Mainz widmen sich in einem weltweit einzigartigen Projekt der Etablierung "ergebnisloser" Arbeiten als Meilensteinen verantwortungsvoller Forschung.
*http://www.stifterverband.org/wissenschaft_und_hochschule/hochschulperle/2011-04/index.html, 01.04.2011*

Vom Sinn des Nullresultats: Mainzer Doktoranden gründen eine ungewöhnliche wissenschaftliche Zeitschrift.
*Frankfurter Allgemeine Zeitung, 08.03.2011*

"Erfolg hat viele Väter, Misserfolg ist ein Waisenkind", sagt das Sprichwort. Der Stifterverband für die Deutsche Wissenschaft hält nun dagegen: Er zeichnet eine als einmalig bezeichnete Wissenschaftszeitschrift aus, die sich mit erfolglosen Forschungen und Versuchen befasst, das an der Johannes Gutenberg-Universität Mainz herausgegebene "Journal of Unsolved Questions".
*http://www.rhein-zeitung.de/startseite_artikel,-Zeitschrift-ueber-Pleiten-in-der-Wissenschaft-geehrt-_arid,227794.html, 01.04.2011*

Lizenz zum Scheitern – Aus Misserfolgen lernt man am besten, finden zwei Doktoranden.
*www.zeit.de/campus/2011/04/forschung-misserfolge, 22.06.2011*

Wissenschaftler unter Publikationsdruck - Warum Forscher Fehlversuche verschweigen. Unklare Forschungsergebnisse sind nicht gefragt. Das führt sogar zu Datenfälschungen.
*Frankfurter Rundschau, 03.05.2011*

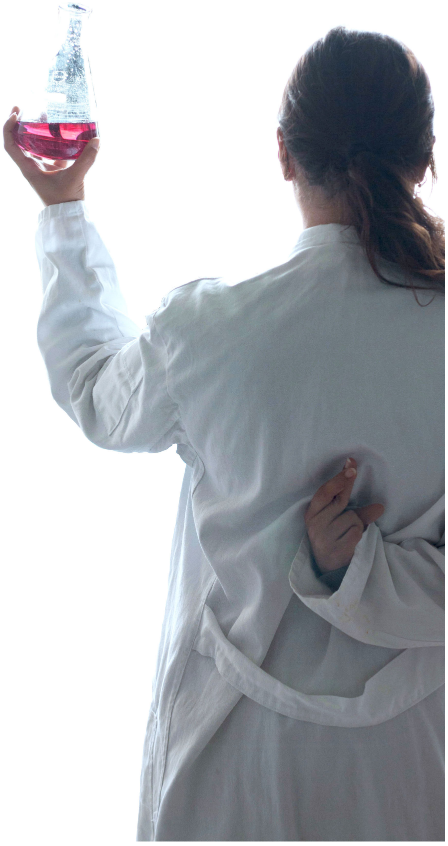
Während der Sache sicherlich eine gute Idee zugrunde liegt, bezweifle ich irgendwie, dass sie Erfolg haben wird. Warum sollte jemand seine Fehlschläge publizieren? Ja, sicherlich könnten die Informationen für andere Forscher nützlich sein - andererseits setzt man sich dadurch potenziell Spott aus, vor allem in der "westlichen Welt" und kann so eventuell vor Kollegen schlechter dastehen.
*Comment on www.zeit.de/campus/2011/04/forschung-misserfolge by DetlevCM , 22.06.2011*

The Journal of Unsolved Questions, online in Mainz, Germany, seems well worth a look. It points towards things that are deep at the heart of science (and of, well, everything).
*http://improbable.com/2011/03/02/the-journal-of-unsolved-questions, 02.03.2011*

Wenn Forscher und Wissenschaftler versagen, bekommt das in der Regel niemand mit. Regelmäßig geht etwas daneben, nur allzu oft sind Forschungsergebnisse ein Fall für den Papierkorb. Scheinbar. Ein neues Fachmagazin, das "Journal of Unsolved Questions", will diesem Denken entgegenwirken. Eine Recycling-Tonne, die jeder durchwühlen kann.
*http://www.n-tv.de/wissen/Wenn-Forscher-im-Muell-wuehlen-article3478816.html, 06.06.2011*

Why scientists should foucs on questions rather than results.
*http://www.young-germany.de/nc/news-verwaltung/news-singleview/article/why-scientists-should-foucs-on-the-question-rather-than-the-answer.html, 28.04.2011*

# Honesty in Science - Interview with Ombudsman for Science Prof. Dr. Siegfried Hunklinger



In 1997, one of the biggest cases of scientific misconduct in the history of medicine was uncovered. Eberhard Hildt, co-worker of the esteemed cancer researchers Friedhelm Hermann and Marion Brach, turned to his former Ph. D. advisor Peter Hans Hofschneider asking for help. He had noted obvious irregularities in his new lab that could only be due to fraudulent behaviour. In the end, it turned out that in 94 publications Hermann and Brach had committed forgery.
As a reaction to the scandal, the Deutsche Forschungsgemeinschaft named a commission on professional self regulation in science. The commission's recommendations included establishing a team of ombudsmen for science, to whom scientists can turn in case they observe scientific misconduct. One of them is Siegfried Hunklinger, a former professor for physics at Ruprecht-Karls University, Heidelberg. He held the office of an ombudsman from 2005 until May 2011. In May, he was succeeded by Katharina Al-Shamery, professor for chemistry at the Carl-von-Ossietzky University in Oldenburg. More information about the ombudsman can be found at http://www.ombudsman-fuer-die-wissenschaft.de/
We talked to Prof. Hunklinger about his work as an ombudsman and about recent developments in scientific conduct.

**JUnQ:** Professor Hunklinger, you are Ombudsman for Science. What does an ombudsman do?
**Hunklinger:** Scientists may contact the Ombudsman if they are involved in a dispute concerning good scientific practice. When someone approaches us with a problem, we try to do justice to both sides. We do not judge, instead we mediate.
**JUnQ:** Can you give an example on how you mediate?
**Hunklinger:** First, we ask the whistleblower, who contacted us with a complaint, to describe the issue in written form. This already helps us to understand what the issue is about. However, there is always an opposite party, the accused person, whom we also interview. The truth often lies between both views. Usually, we can solve many problems on the basis of the two written statements because we understand what the problem is and on whom to put the bigger portion of the blame, if it is even appropriate to speak of blame. Next, we propose a solution. For instance, if the authorship of a publication is controversial, one can add further authors or change the acknowledgment. In many cases, an agreement is achieved in this way. If this does not work, we summon both parties to a hearing. It sometimes helps just to talk to each other. This kind of mediation also often leads to an agreement. The most unpleasant case is that data are evidently counterfeited or manipulated. This is beyond our means. We will inform the appropriate institutions, for example the Deutsche Forschungsgemeinschaft or the Max-Planck-Gesellschaft. These institutions are in charge of imposing sanctions, we only mediate.
**JUnQ:** How many cases are there per year and of what kind are they?
**Hunklinger:** There are approximately 50 to 60 cases per year. Most of them concern disputes over the authorship of publications. Besides that, there are plagiarism allegations, counterfeits, and disputes with journal publishers. Bullying is noteworthy as well. Scientists in leading positions often put pressure on people that are not liked for some reason. This can cause severe misconduct.
**JUnQ:** If one looks at the great scientific scandals like the ones involving Jan-Hendrik Schön and Hwang Woo-suk, one question comes to the mind: Why do scientists do this and what drives them? Do you have an answer to this question?
**Hunklinger:** No, actually not. Concerning Schön, I can understand him a little bit. He was at the beginning of his career and wanted to reach the top. The path he pursued was fantastic. If people had not realized the fraud, he would have become director of a Max-Planck institute and things

would have turned out well for him. Concerning Hwang, I do not understand him. He was a well-recognized scientist. For example, he cloned dogs and he did excellent science after the scandal. It is incomprehensible to me why he faked results in the meantime. The pursuit of becoming famous cannot be the reason as he was already famous. Maybe I lack the right mindset to understand this case.

**JUnQ:** What are appropriate means to prevent such cases of fraud?

**Hunklinger:** We are not able to make it impossible, this is hopeless. However, we can improve the system if young scientists resist fraud and if they do something against it. For example, they should contact an ombudsperson to get advice. This does not have to be the Ombudsman for Science, there are also local ombudspersons.

**JUnQ:** Do you think that the self-control mechanisms in science are sufficient to unveil fraud in its early stages?

**Hunklinger:** I do not consider them to be sufficient. There will always be scandals, we cannot completely avoid them. But I neither consider external control mechanisms helpful, scientists are normal people.

**JUnQ:** Science is much more regulated than 50 years ago. People often regret that scientific freedom is curtailed and that scientists spend a lot of time doing administrational work. Do you think there is a connection to scientific misconduct? Is there too much regulation rather than too little?

**Hunklinger:** I'd like to agree, science was much freer 50 years ago. There was no pressure to publish as many articles as today. It was not necessary to create a publication out of every tiny result. This benefited science and we should try to get back to that state. But it is a long way.

**JUnQ:** There are public efforts to measure the quality of research and make research transparent to society. Hirsch indices and impact factors are often employed for that purpose. Do you think there is another way?

**Hunklinger:** To be honest, I have a low opinion of these measuring numbers. Things may have changed, but in my days, the situation was as follows: When someone was appointed to a professorship, everybody knew that this was a good man without checking indices that have a random nature. In my opinion, the important thing is to talk to the people concerned. This will lead to reasonable decisions.

**JUnQ:** Professor Hunklinger, we thank you for the interview.

– Thomas Jagau and Leonie Mück

## Book Review: Plastic Fantastic - How the Biggest Fraud in Physics Shook the Scientific World

*Eugenie Samuel Reich, author of the book "Plastic Fantastic" about one of the most outrageous cases of scientific misconduct of all times involving German-Austrian physicist Jan Hendrik Schön*

"He looked just like you and me. Just like everybody else. Who would have thought that he'd be capable of such things...? ", was Bob Cava's first comment when we got to talk to him about Jan Hendrik Schön, the person whose name stands for one of the biggest and most sensational cases of scientific fraud in the history of science. Prof. Cava was a colleague of Jan Hendrik Schön at Bell labs before he took on a professorship at Princeton University and saw him coming and going to his lab, working on his computer, having his lunch break. "Who would have thought that he'd be capable of such things" – this phrase awkwardly sounds familiar, but not from the context of science. Rather it is connected with one's favourite crime and mystery show or with reading the latest detective story. A normal looking man coming to mess up your world, threatening security and defying rules and laws – this is superb material for the next episode of "Tatort" or "Criminal Minds". Indeed, Eugenie Samuel Reichs book about the Schön scandal reads like a documentary of a scientific crime. Jan Hendrik Schön, a postdoc from Konstanz, Germany, arrives at the prestigious Bell Laboratory run by AT&T in January 1997 to work on field-effect transistor experiments using organic crystals. Expectations are high, the supervisor, Bertram Batlogg, wants to prove that he can do more than high temperature superconductivity – the topic that he had gained a splendid reputation for. But getting hands on such a new and experimental field is hard and laborious, so Jan Hendrik Schön commits the worst crime possible in science: He falsifies data. No ingredient for a good crime story is missing: There is the criminal, Jan Hendrik Schön. There are his victims: Supervisors, whose names got stained by the fraud, on the one hand, and Ph. D. students, whose careers got ruined because they unsuccessfully tried to replicate his experiments, on the other. And there are detectives, skeptical scientists like nobel prize winner Robert Laughlin, who doubted the credibility of Schön's claims and who finally tracked down duplicated data in his publications in 2002. But Reich is well aware that crimes you observe in reality are far more complex than crimes on TV. Who really is a victim and who is a wrongdoer? Shouldn't Schön's co-authors and supervisors take blame for being starry-eyed and deprived of judgment by the wish of getting a piece of Schön's cake? Reich's account of the case is therefore connected with a detailed study of the scientific community. Trying to explain how Schön could falsify data for almost five years without anyone proving him wrong, she does not only consider Schön's character and intrinsic motivation. Reading about the competitive environment at Bell Labs, the "Publish or Perish" imperative and how scientists are "slaves to publication", the difficulty of whistleblowers to allege a fellow scientist guilty of fraud, and the lack of communication among the "detectives", gives a realistic account of the way science nowadays works. But the author frames this comprehensive account with the following question: Is the Schön scandal the story about how science succeeds in self-correcting? Or is it a story about how it fails? In my opinion, this is not the most important question to be asked about the case. The fraud eventually came to light and, taking into account how sensational Schön's claims were, it would have been detected in any way. Science is definitely self-correcting if the claims at question are important enough. I think the Schön scandal poses a different and far more problematic question. Before getting persecuted for fraud, Jan Hendrik Schön was the embodiment of a successful scientist. He was so highly celebrated that the Max-Planck Society intended to appoint him to become the youngest director of a Max-Planck Institute ever. His work was full of sensational claims, maybe not claims that revolutionized physics but achievements that everybody predicted to be accomplished in the near future and they were all accomplished by Schön. In 2001 alone, he published 17 papers in the journals Nature and Science, only occasionally writing technical, full papers to describe in detail what he did for fellow scientists. His research strolled along like a mystery, like a dream coming true. When Horst Ludwig Störmer, nobel prize winner and director of Bell Labs until 1997, was confronted with the lacking reproducibility of Schön's work, he supposedly said: "Hendrik has magical hands!" – as if this could explain everything. The scientist appears as a brilliant magician, magically waving his hands to achieve what the world has been waiting for. Such a character splendidly fuels the drama in a good crime story, with the criminal as a bewitching wunderkind without morale. But is this really the character that we want to conventionalize as the prototype scientist? Why do we ignore what science really is, namely hard work, frustration, failure, and confusion? It is the wishful thinking, the gap between ideal and reality, the masquerade in science that is impressively demonstrated by the Schön case. And it is this wishful thinking that blinded supervisors, publishers, referees, and colleagues of Jan Hendrik Schön and made them overlook his flaws. Like a good crime show, the danger of getting blinded like that should haunt every scientist's sleep, waking him up at night shivering from the fear of losing their objective judgment to a magician. And although Eugenie Reich suggest a different interpretation of the Schön scandal, this page-turning tension grows with every new details on poor judgment and human weakness that she provides.

*Eugenie Samuel Reich, "Plastic Fantastic - How the Biggest Fraud in Physics Shook the Scientific World", Macmillan Publishers 2009, ISBN-10: 0-230-22467-9*

–Leonie Mück

# Interview with Prof. Dr. Gerhard Fröhlich on the Schön Scandal: "Self control mechanisms are a myth in science to avoid any serious external control"


*Prof. Dr. Gerhard Fröhlich (third from left) during the panel discussion on the topic "Publish or Perish. . . ? " (Mainz, May 23rd). Other debaters (from left to right): Dr. Peter Gölitz, Editor-in-Chief of "Angewandte Chemie", moderator Jan-Martin Wiarda, Editor of DIE ZEIT, Prof. Dr. Gerhard Fröhlich, Prof. Dr. Katharina Al-Shamery, ombudsman of Science in Germany*

The Schön case has not only been widely discussed by journalists and media but is also of interest to researchers working in the field of theory of science. Prof. Dr. Gerhard Fröhlich from the Johannes-Kepler-University, Linz, is one of them. His main research areas are the theory of culture and media and philosophy of science, especially scientific communication and scientific misconduct. Prof. Fröhlich came to Mainz for the panel discussion "Publish or Perish. . . ?" and the Journal of Unsolved Questions interviewed him about the Schön scandal and the book "Plastic Fantastic" during that visit.

**JUnQ:** Almost 10 years have passed since Jan Hendrik Schön's fraud was discovered. What has happened in the scientific community since then to prevent fraud?
**Fröhlich**: First of all, it is hard to consider the "scientific community" in its unity, since national styles and policies as well as the individual scientific disciplines differ greatly. In disciplines where staggering, high profile scandals occurred in the last years, some provisions are noticeable.

Regarding medical research, the institution of "honorary authorship" has been impeded. Now, when a medical article is to be published, every single contributor should be assigned to a specific contribution. In some journals, the authors even have to sign personally that they endorse the methods and outcome of the study. In the field of medicine, research registers have been implemented with the goal to prevent the disappearance of disagreeable results. In medical research, 40 to 60 percent of studies never get published because they fail to produce the desired outcome. Unfortunately, these research registers are still far from listing all studies and all important details of the covered studies.

In other areas, where the public is less interested in reliable results, provisions against plagiarism, fraud, and deception are still rather lax. This starts with the lack of any legal basis to penalize cheating during exams in Austria and ends with missing declarations under penalty of perjury – for example in case of Karl-Theodor zu Guttenberg and the Bayreuth affair.
**JUnQ:** Eugenie Samuel Reich frames her account of the Schön scandal with the question if the Schön case is an example of functioning self-correction mechanisms in science – or if it is an example for the opposite. What is your opinion?
**Fröhlich:** Self control mechanisms are a myth in science to avoid any serious external control. I have studied all fraud affairs precisely and in almost every case anonymous allegations coupled with mass media outrage – in most recent years with an interim period of outrage on the internet – were necessary before the institutions themselves agreed to take action. In the US, the first serious sanctions against scientific fraud were imposed from politics against the grim resistance of scientists. The role of a certain Albert Gore should not be forgotten.
**JUnQ:** Why could Schön publish fake data for such a long time? Which protagonists failed to notice?
**Fröhlich:** Science and its sponsors, media and politics, everybody wants heros, "Übermenschen". The lion's share of uncovered scientific cheaters were supermen or superwomen, shooting stars in their field, decorated with honors and predicted to win the Nobel Prize. In every case, though, an elderly gentleman held his protective hand over them to award them an official seal of scientific credibility.

With Schön it was Batlogg, in the Korean clone scandal it was US scientist Schatten, in the German cancer research scandal it was Mertelsmann. Not one of them was subject to prosecution after the fraud had been detected, although they were co-authors and, in case of Batlogg, even corresponding authors on a long list of falsified studies. A long publication list is well known to be hard cash in science, therefore the senior mentors heavily profited from the falsifications.

Besides the mentors, project managers, and research institutions, the scientific journals malfunctioned, of course, especially Science and Nature, journals with a general scope. Generally, refereed journals are a bit dishonest: In the past they claimed that they hardly encountered any fraud, plagiarism, and deception because their reviewing system worked so well. Now, after countless cases of fraud, they claim that peer reviewing and the journal business have never been responsible to detect and avoid scientific misconduct.

**JUnQ:** Eugenie Reich's book heavily focuses on the figure Schön as the criminal and mastermind. She portrays the institutions and the scientific community as the protagonists that could not prevent the fraud. Do you think that this perception does justice to the case?

**Fröhlich:** Personalizing and scandalizing have always been a strategy to acquit science from structural failures, attributing all problems to the criminal actions of individual delinquents. They are put forward as scapegoats to clear science. Mrs. Reich's personalized and scandalized perception of the case relies on second-hand statements about conversations, impressions, and events 10 or 20 years ago. She claims that her interview partners remembered everything correctly, but I highly doubt their statements. In the retrospective, it is always easy to reinterpret events in a way that put the blame on one individual only.

**JUnQ:** In her book, Eugenie Reich quotes a whistleblower, who accused colleagues of scientific misconduct. He states that after his allegation of the fraud he wanted to stay anonymous for the rest of his life "like a rape victim". Why do accusations weigh so heavily on whistleblowers?

**Fröhlich:** As a matter of fact, the protection of whistleblowers still is not nearly sufficient yet. Reviewers are allowed to remain anonymous, but activists in the German plagiarism wikis are attacked because they do not reveal their identity. Peer Review is anonymous, too - but almost nobody is critizising the arcane practices of scientific funds and journals. Together with two colleagues, I founded the "Initiative for Transparency in Science" in Austria[1] in order to enhance scientific ethos in Austria, which was a cause for aggressive anonymous mail addressed to me.

**JUnQ:** The Schön scandal caused a big outrage in the scientific world. But what about the small data embellishments and the day-to-day inaccuracies in the lab? Are we doing enough to prevent fraud at its early stage?

**Fröhlich:** Science will never be completely faultless. There will always be fraud, deception, and plagiarism. But individual states, research institutions, scientific associations, scientific journals, and so forth, should have the power to make more effective provisions. Tighter legal arrangements would also be necessary. I think it is outrageous that ghostwriter offices can freely prosper without the possibility to prosecute them legally. One of the bigger ones praises itself with the authorship of 5000 projects in the German speaking countries in the last seven years. All beneficiaries of falsifications should be held accountable for the misconduct and should return their gains. These could be invested in a trust for the detection of falsifications, because sometimes only a few thousand Euros are lacking for the prosecution in certain cases. In Germany there is an additional overcast perception of "scientific freedom". For example, a scientist from Gießen successfully went to court against the appointment of a commission investigating possible scientific misconduct in his lab. He won the case with the argument of "scientific freedom". Another aspect, that some publishers probably are not so happy about, is Open Access, meaning the barrier-free access to all scientific publications and data. Without this, the "collective intelligence" of all scientists and journalists does not have any effect. As long as publications are subject to so many legal stipulations that they can neither be handled nor analyzed by search engines, scientific misconduct will keep on prospering.

Further reading:

*Gerhard Fröhlich: Visuelles in der wissenschaftlichen Kommunikation - z.B. Betrug und Fälschung, 2003. In: European Journal for Semiotic Studies 15 (2-4), 627-655. (Issue on "Iconicity", ed. by Jeff Bernard and Gloria Withalm), http://eprints.rclis.org/archive/00011693/*

–Leonie Mück

## Questions of the Week

*The Journal of Unsolved Question presents a "Question of the Week" on its homepage every week. Set up and formulated by the members of the editorial board, the main purpose of the "Question of the Week" consists in intriguing the reader by presenting topics of ongoing research. "Questions of the Week" published so far cover a wide variety of scientific fields, but share the feature to be of certain importance to several disciplines.*

*In the following, we present selected "Questions of the Week" from the last six months.*

### Are there smooth and globally defined solutions to the Navier-Stokes equations?

*by Thomas Jagau*

Although first formulated in the 19th century, our knowledge of the Navier-Stokes equations remains minimal. These basic equations of fluid mechanics describe gas and liquid flow and can be derived by invoking conservation of momentum, mass, and energy for a continuum fluid. They form a set of nonlinear partial differential equations of second order, for which it has not been mathematically proved yet that smooth and global solutions always exist in three dimensions. Understanding the Navier-Stokes equations is also considered as a first step towards gaining better insight

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into the phenomenon of turbulence. In spite of the great importance for science and engineering, the Clay Mathematics Institute ranks this question among the seven most important open problems in mathematics and has offered a USD 1,000,000 prize for a solution or a counter-example.

Read more: http://www.claymath.org/millennium/Navier-Stokes_Equations/navierstokes.pdf

## Comment on: Are there smooth and globally defined solutions to the Navier-Stokes equations?

*by Helmut Z. Baumert*
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You correctly state that behind this Question of the Week is the search for a solution to the turbulence problem. Maybe, its solution contributes one day to the solution of the turbulence problem, but I am skeptic. Solving the turbulence problem means finding possibly unknown laws of mixing of momentum and scalars at asymptotically high Reynolds numbers. About one hundred years ago, Osborne Reynolds, soon thereafter also Friedman and Keller, and later their many followers thought that we can solve the problem by series expansions of the Navier-Stokes equations, a process which provides dynamic equations of motion for higher and higher statistical moments. Unfortunately, the expansion does not visibly converge, certain closure assumptions are needed so that this approach is not strict. Another historical aspect is that, due to more attractive problems like fission, fusion, semiconductors etc., physicists lost their interest in turbulence at an early stage. So, this topic became a field of activity for engineers and mathematicians. With respect to theory, they all followed – more or less – the aforementioned paradigms of Reynolds, Friedman, and Keller – without any exact result. E.g., in the famous textbook of Landau and Lifshitz, we can still find a statement that universal constants of turbulent motion, like von Karman's constant, can only be measured rather than predicted by theoretical considerations.
An exception was Kolmogorov who realized the hopelessness of the aforementioned paradigms and introduced an ad-hoc argument: similarity analyses, which immediately led to the prediction of the scaling laws of turbulent spectra, e.g., the famous $\frac{5}{3}$-law, which is strict. At infinitely high Reynolds number the physical properties of the specific fluid under study "vanish", i.e. a vanishing viscosity is observed. This sort of turbulence is consequently governed by the regularized Euler equation, which represents pure "inert geometry". Therefore a new (2005, 2009, 2010) attack against the turbulence problem rests on the Euler equation and its singular solutions, so-called "vortex atoms" that were first introduced by Lord Kelvin almost 150 years ago based on von Helmholtz vortex theorems. They can be treated as non-trivial three-dimensional particles in motion. In most cases, these motions are extremely hard to predict and thus, a special branch of mathematics – topological hydrodynamics focuses on them today. But there are two exceptions: completely isolated vortices, and a "gas" of very many vortices. The former case is trivial. In the latter case, one can do what has already been done by Maxwell in his kinetic theory of gases, which is a special case in the field of more general many-particle problems: assume chaotic, i.e. Brownian motion of molecules or atoms. This new paradigm applied to a gas of vortex couples leads us to simple and comfortable equations of motion of the advection-diffusion-reaction typ) for the key variables of turbulence, i.e., for turbulent kinetic energy and root mean square vorticity. Details can be found here: http://arxiv.org/abs/0907.0223

The approach even allows for a prediction of von Karman's constant as $\frac{1}{\sqrt{2\pi}} = 0.399$. The international standard value based on measurements is 0.4. We see that the solution of the turbulence problem and the Question of the Week on the Navier-Stokes equations are possibly not related at all. Maybe in the far future the question can be solved and a link to the turbulence problem can be established. But at least today, only the vortex-particle paradigma sketched above has "predicted" some of the fundamental constants of turbulent motion in sufficient accuracy.

## Why are there more boys than girls around Gorleben and Asse?

*by Christian Ludwig*

In the vicinity of the German nuclear waste storage site Gorleben, significantly more boys than girls have been born since the commissioning in 1996. The situation is similar around the nuclear waste storage site Asse. For instance, between 1971 and 1979, 121 boys and 85 girls have been born in Remlingen.

Of course, some people claim that radioactivity is the reason for this asymmetry. But what exactly does "significant" mean? In physics, data are considered significant if they deviate more than 3 sigma from the expected value. If we allow a deviation of only 2 sigma from the expected value, 121 and 85 are not significant. Of course, these are only two numbers and there are more data that we have no access to.

What speaks against a causal connection is the fact that no one has the slightest idea how it could be explained physically. Measurements did not uncover any unusual radioactivity around Gorleben. However, it cannot be denied that some peculiarities have been observed near the German nuclear waste storage sites. But could it be that they were only found that abundantly, because people were specifically looking for them?

We do not know the answer, but if the increased birthrate of boys is more than pure coincidence, there is no proof for the reason to be radioactivity from the storage sites. The cause stays a mystery.

Further reading:

http://www.ndr.de/regional/niedersachsen/heide/gorleben687.html

http://www.ndr.de/regional/niedersachsen/harz/asse563.html

Picture: The Gorleben exploration mine

## How does glatiramer acetate modify the autoimmune mechanisms in multiple sclerosis?

*by Johannes Heymer*

Multiple sclerosis is a chronic desease that often leads to severe neurologic defects by an autoimmune process which results in demyelination. It is among the most common causes of disability in young people in Europe. A lot of aspects of the pathophysiology of multiple sclerosis have not been unterstood yet. There are many different concepts for the therapy of multiple sclerosis, most of them are based on immunosupression or direct immunomodulation by the so called "biologicals‘. In contrast to those concepts, glatiramer acetate is just a simple mixture of amino acids. Different mechanisms have been discussed, e.g. that glatiramer acetate binds to effector cells of the immunosystem or that it changes the ratio of different types of t-cells. Which mechanism dominates the therapeutic benefits resulting from a therapy with glatiramer acetat has not been explained.

## Why the predominance of silica spicules in marine sponges?

*by Rute André*

Sponge spicules are between some of the most studied biomaterials nowadays, and depending on the species they can be made of silica (Demosponges and Hexactinellid) or calcium carbonate (Calcarea).
This different classes have, of course, different habitats and the presence of either a calcium carbonate or silica spicule endoskeleton can be partially justified by the local environment (deeper vs. shallower waters, for example). Nevertheless, sponges with silica spicules are far more abundant than calcarea sponges (about 90% higher). When you look at it, silicon (or silicic acid as it appears usually in the sea) concentrations in sea water are quite lower than that of calcium. Besides in an evolution point of view, most skeletons present nowadays are composed of biomaterials with calcium (corals, shells, hydroxyapatite in human bone, for example).

So the question regarding the predominance of sponges with silica spicules still leaves room for debate, with several different opinions like the simple natural selection regarding the fact that in deeper waters where the silica containing sponges are more dominant, there are less predators in opposite to the shallower waters where sponges containing calcium carbonate spicules are generally more proliferous. Other opinions focus on the evolution of highly effective mechanisms of transport and accumulation of silicon intracellularly which allowed the taxa to establish successfully in a small niche.

Further reading:
http://geology.geoscienceworld.org/cgi/content/abstract/25/4/303
http://www.ncbi.nlm.nih.gov/pubmed/15128286

## Is it possible to create magnetic semiconductors that work at room temperature?

*by Yuriy Khalavka*

Magnetic semiconductors are semiconductor materials that exhibit both magnetism and semiconductor properties. Magnetic semiconductors, which can be formed by doping or alloying semiconductors with suitable transition metal ions (e.g. Mn), have potential applications in spin electronics, as they provide a simple way to combine spin dependent phenomena with conventional semiconductor operation. Therefore, the study and development of such ma-

terials and the origin of ferromagnetic order in systems with low carrier densities and low concentration of magnetic ions, found both in semiconducting and metallic systems, is presently investigated in many laboratories. [1] For those materials optically-induced magnetization and magnetically sensitive optical and electrical properties have been demonstrated at low temperatures but not yet in a range warm enough for real applications. [2,3]
One of the ways to increase the working temperature of such materials is to create nanopatricles out of magnetic semiconductor material. Despite some successes, many of these efforts have failed, for reasons that remain unclear. For example, Mn was incorporated into nanocrystals of CdS and ZnSe, but not into CdSe and CdTe -despite comparable bulk solubilities of near 50 per cent [4]. These difficulties, which have hindered development of new nanocrystalline materials, are often attributed to 'self-purification', an allegedly intrinsic mechanism whereby impurities are expelled. So if magnetic semiconductors that work at room temperature will be created is still open question.

References:

1. http://www.mpg.de/
2. Appl. Phys. Lett. 83, 3575, (2003)
3. Appl. Phys. Lett. 84, 3337, (2004)
4. Erwin, S. C. et al. Nature 91, 436, 2005

## How does a queen bee become royal by epigenetics?

*by Leonie Mück*

Female bee workers and bee queens share exactly the same genome. Nevertheless, there phenotypes differ dramatically: The queens bee's abdomen is longer and – more importantly – she is the only sexually mature and reproductive female in one hive.
The bee workers select special larvae to become queens and feed them with a distinct amount of royal jelly. The special nutrition ignites a cascade of reactions leading to epigenetic effects, namely the methylation of some DNA sequences. The methyle groups change gene expression and can in part explain the behavioral and reproductive differences between the workers and the queen. Recently, scientists from the German Cancer Research Centre in Heidelberg, Germany, and the University of Canberra, Australia, discovered that more than 550 genes in the queen's genome show a different methylation pattern than the workers'.

The methylation agglomerates in regions of the genes, where splicing – the process where the gene's introns are removed – occurs. The authors conclude that the methylation may influence the splicing process therefore generating the queen's distinct gene products. But how exactly the bee is crowned queen by epigenetics remains an open question.

Read more:

F. Lyko, S. Foret, R. Kucharski, S. Wolf, C. Falckenhayn et al. (2010), The Honey Bee Epigenomes: Differential Methylation of Brain DNA in Queens and Workers. PLoS Biol8(11): e1000506. doi:10.1371/journal.pbio.1000506

Picture: The adult queen bee (picture by Pollinator)

# Articles

## On the Fermionic Shadow Wave Function and Novel Attempts to Solve its Sign Problem

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We present the Fermionic Shadow Wave Function in the context of variational quantum Monte Carlo for disordered systems. Using the example of liquid $^3$He it is demonstrated that this allows for very accurate calculations, but due to its sign problem only for small systems. For this reason two novel methods are proposed that in principle solve the associated sign problem, but do not allow for realistic simulations yet.

The difficulty to solve the Schrödinger equation for many interacting particles is due to the fact that it is in general impossible to analytically solve it for more than a few particles. Variational Monte Carlo (VMC) [1] is a stochastic method which allows to find the ground-state solution of the many-body Schrödinger equation. The main ideas underlying VMC are the application of the variational principle and the use of importance sampling Monte Carlo to efficiently evaluate the high-dimensional integrals of many different expectation values and in particular the energy [1]

$$E = \frac{\int dR\, \psi^*(R) H \psi(R)}{\int dR\, \psi^*(R)\psi(R)} \,. \tag{1}$$

Since many-particle correlation effects are included by the use of a so-called trial wave function, VMC is substantially more accurate than commonly used mean field methods and permits to treat even strongly correlated systems. From the outset the exact trial wave function is unknown and needs to be approximated. However, due to the fact that adding a simple correlation function, such as the Jastrow correlation factor, permits to recover most of the dynamic correlation, in many cases VMC gives excellent results.

Here we consider the Shadow Wave Function (SWF), first introduced by Vitiello, Runge and Kalos,[2] as our trial function. The SWF allows to describe all possible condensed phases (gas, liquid and solid) and even phase coexistence [3] within the same functional form. As a consequence, it is for instance possible to simulate a solid without explicitly defining its crystal structure, which instead emerges from the calculation. In fact, with the SWF it is even feasible to describe inhomogeneous systems.[4-6] Moreover, the SWF has further very appealing properties, e.g. it introduces correlation of any order and obeys a strong similitude with the exact bosonic ground state wave function.

The general form of the SWF takes the form

$$\psi_{\text{SWF}}(R) \equiv \psi_p(R) \int dS\, \Xi(R,S)\, \psi_s(S) \,, \tag{2}$$

where $S$ are auxiliary degrees of freedom called shadows, $\psi_p(R)$ and $\psi_s(S)$ are Jastrow functions that describe the correlation between the particles and between the shadows respectively, while $\Xi(R,S)$ is a kernel that correlates the particles with their shadows. Neglecting, for the moment, the requirement of antisymmetry necessitated by the Pauli exclusion principle, typical choices are

$$\psi_p(R) = e^{-\frac{1}{2}\sum_{i<j} u_{pp}(r_{ij})} \tag{3a}$$

$$\psi_s(S) = e^{-\sum_{i<j} u_{ss}(s_{ij})} \tag{3b}$$

$$\Xi(R,S) = e^{-\sum_{i=1}^{N_p} u_{ps}(|\mathbf{r}_i - \mathbf{s}_i|)} \,, \tag{3c}$$

where $u_{pp}$, $u_{ss}$ and $u_{ps}$ are the so-called two-body pseudopotentials, since they have a role similar to the potential in the Boltzmann distribution. Although it is possible to include three-body and even higher order terms, for the sake

[1] We use the notation $R \equiv (\mathbf{r}_1, \mathbf{r}_2, \dots \mathbf{r}_N)$ and $S \equiv (\mathbf{s}_1, \mathbf{s}_2, \dots \mathbf{s}_N)$.

of simplicity they are not considered here. In any case the SWF not only maintains the translational properties of the gas and liquid phases, but through the kernel also enables the necessary localization to accurately describe the solid phase. In fact, for densities at which the system is experimentally found to be in the solid phase, the variationally optimized parameters yield a localization of the shadows in the correct crystal structure. The real degrees of freedom are in turn localized near the corresponding shadows by the kernel.

In a few studies, the SWF has been successfully applied to bosonic systems, in which the wave function is non-negative.[3,7-10] However, due to the aforementioned antisymmetry requirement, the extension to fermionic systems is nontrivial and gives rise to a sign problem. Generally, an efficient and rigorous method to simulate fermionic systems therefore remains an open and most challenging problem.

The extension of the SWF to fermionic systems, where the wave function is real but equally positive and negative, is established in Section 1. The origin and impact of the sign problem will be exposed in Section 2, while in Sections 3 and 4 we are going to present and discuss in depth two novel attempts to solve it.

# 1 The Shadow Wave Function for Fermions

As fermions obey Fermi-Dirac statistics, an antisymmetric version of the SWF is required, that must change sign upon interchange of any two fermions in order to comply with the Pauli exclusion principle.

The simplest way to achieve this, is to adjoin the Jastrow correlation factor with a Slater Determinant (SD) that depends on the particle positions $R$. We will call this the Antisymmetric Shadow Wave Function (ASWF) [8]

$$\psi_{\text{ASWF}}(R) \equiv \det(\phi_\beta(\mathbf{r}_\alpha))\, \psi_p(R) \int dS\, \Xi(R,S)\, \psi_s(S)\,, \tag{4}$$

where $\phi_\beta(\mathbf{r}_\alpha)$ are the orbitals that represent the SD. In order to preserve the translational symmetry of the wave function, which is one of the many appealing properties of the SWF, plane wave orbitals are the natural choice.

Another possibility is to introduce a SD built up of orbitals as a function of shadow positions $S$. The resulting Fermionic Shadow Wave Function (FSWF) then reads as:

$$\psi_{\text{FSWF}}(R) = \psi_p(R) \int dS\, \Xi(R,S)\, \det(\phi_\beta(\mathbf{s}_\alpha))\, \psi_s(S)\,. \tag{5}$$

It is possible to demonstrate that, just as the ASWF, the FSWF is antisymmetric upon particles exchange.[11] But since the latter furthermore provides [12] (i) a closer similitude with the projection onto the exact fermionic ground state (no one actually knows how the propagator on the lowest antisymmetric state behaves), (ii) the correct asymptotic nodal structure and (iii) naturally includes backflow effects,[13] the FSWF rather than the ASWF is to favor.

As can be seen in Table 1, applying the FSWF to the liquid phase $^3$He provides much improved variational energies, even though only for a rather small system with $N = 38$ particles and with an admittedly larger statistical uncertainty. [2] In fact, as we are going to explain in detail in the next section, the FSWF entails a serious sign problem that makes it essentially impossible to obtain reliable results whenever $N > 38$. This limitation on the size of the system not only reduces the applicability, but also the reliability of the FSWF, due to fairly large finite-size effects. Therefore, it would be desirable to solve, or at least alleviate, the sign problem and allow for even more accurate simulations with many more particles. In order to approximately compare the various energies for different values of $N$, from now on, we shall refer to the energy per particle, denoted as $\mathcal{E}$.

| Trial Function | $\mathcal{E}$ | $N$ |
|---|---|---|
| J-SD | $-1.004 \pm 0.006$ K | 66 |
| ASWF | $-1.222 \pm 0.006$ K | 66 |
| FSWF | $-1.966 \pm 0.035$ K | 38 |

Table 1: The energy per particle of liquid $^3$He is denoted by $\mathcal{E}$, which is obtained by VMC calculations using different trial wave functions. The number of particles is indicated by $N$, while the Jastrow-SD (J-SD) trial wave function is defined as $\psi_{\text{J-SD}} \equiv \det(\phi_\beta(\mathbf{r}_\alpha))\, \psi_p(R)$, where $\phi_\beta(\mathbf{r}_\alpha)$ are plane waves.

# 2 The Sign Problem of the Fermionic Shadow Wave Function

Applying the FSWF causes a serious challenge in the evaluation of the energy, which is indispensable to employ the variational principle. Usually the energy can be estimated by

$$E \simeq \frac{1}{M} \sum_{i=1}^{M} E^{loc}(R_i)\,, \tag{6}$$

where $E^{loc}(R_i) = \frac{H\psi(R_i)}{\psi(R_i)}$ is the so-called local energy and $M$ the number of sampling points. The positions of the particles $R_i$ are sampled from the probability density function (pdf) $\psi^2(R)$, where $\psi$ is the trial wave function. As a consequence, the necessary positiveness of $\psi^2(R)$ is satisfied by definition.

Introducing further the shadows, the energy is evaluated as

[2] We consider an unpolarized 3D system of $^3$He at a density equal to 0.016588 Å$^{-3}$ (liquid phase) using the Aziz potential HFDHE2 [14,15] and periodic boundary conditions in order to mimic an essentially infinite system. We remark that whenever a SD with orbital made up of plane waves is used, the occurrence of a drift (i.e. $\sum_\beta \mathbf{k}_\beta \neq 0$) as well as anisotropy has to be taken explicitly into account. The simplest remedy is to consider only magic numbers for $N$, i.e. numbers that fill the momenta shell. For a 3D system they are: 1, 7, 19, 27, 33, ...

[3] We use the obvious notation $\psi_{\text{SWF}}(R,S) = \psi_p(R)\, \Xi(R,S)\, \psi_s(S)$.

3

$$E = \frac{\int dR\, dS_1 dS_2\, \psi_{\text{SWF}}(R,S_1) H \psi_{\text{SWF}}(R,S_2)}{\int dR\, dS_1 dS_2\, \psi_{\text{SWF}}(R,S_1)\psi_{\text{SWF}}(R,S_2)}\,, \quad (7)$$

so that the corresponding energy estimator can be written as

$$E \simeq \frac{1}{M}\sum_{i=1}^{M}\frac{1}{2}\left(E^{loc}(R_i,S_{1\,i}) + E^{loc}(R_i,S_{2\,i})\right)\,, \quad (8)$$

where $R_i$, $S_{1\,i}$ and $S_{2\,i}$ are sampled from the pdf $\psi_{\text{SWF}}(R,S_1)\times\psi_{\text{SWF}}(R,S_2)$. The average between the $S_1$ and $S_2$ contributions to $E^{loc}$ is introduced in order to accelerate the convergence. Now the positiveness of the sampled function is no more obviously satisfied, since the wave function is evaluated using two different shadows. It is straightforward to see that this problem arises for $\psi_{\text{FSWF}}$, because the SD uses the shadow positions, whereas this is not the case for $\psi_{\text{ASWF}}$. Therefore, it is not possible to sample directly from the pdf $\psi_{\text{FSWF}}(R,S_1)\times\psi_{\text{FSWF}}(R,S_2)$.
However, it is possible to overcome this problem by a simple modification, that is to sample from the pdf $|\psi_{\text{FSWF}}(R,S_1)\times\psi_{\text{FSWF}}(R,S_2)|$ and to introduce the weights

$$\omega_i = \frac{\psi_{\text{FSWF}}(R_i,S_{1\,i})\psi_{\text{FSWF}}(R_i,S_{2\,i})}{|\psi_{\text{FSWF}}(R_i,S_{1\,i})\psi_{\text{FSWF}}(R_i,S_{2\,i})|} = \pm 1\,. \quad (9)$$

The modified energy estimator then reads as

$$E \simeq \frac{\sum_{i=1}^{M}\frac{\omega_i}{2}\left(E^{loc}(R_i,S_{1\,i}) + E^{loc}(R_i,S_{2\,i})\right)}{\sum_{i=1}^{M}\omega_i}\,. \quad (10)$$

Since the sign is now carried by $\omega_i$, the sum in Eq. 10 may be very slowly converging. For disordered systems such as liquid $^3$He studied here this is particularly severe.
Here we have chosen to use the pseudopotentials

$$\begin{aligned} u_{pp}(r_{ij}) &= \left(\frac{b}{r_{ij}}\right)^5 & (11a)\\ u_{ss}(s_{ij}) &= c_1 V(c_2 s_{ij}) & (11b)\\ u_{ps}(|\mathbf{r}_i - \mathbf{s}_i|) &= C|\mathbf{r}_i - \mathbf{s}_j|^2\,, & (11c)\end{aligned}$$

where $V$ is the Aziz potential used in the Hamiltonian, while $b$, $c_1$, $c_2$ and $C$ are variational parameters.
To evaluate the mean value and its unbiased error bar, we have divided the data into $n_{\text{block}}$ disjoint blocks each with its corresponding average value $E_j^{\text{block}}$. It is then possible to calculate the average and the error bar in the following way:

$$\begin{aligned} \langle E\rangle_{\text{block}} &= \frac{1}{n_{\text{block}}}\sum_{j=1}^{n_{\text{block}}} E_j^{\text{block}}\,, & (12a)\\ \sigma^2_{\text{block}} &= \frac{1}{n_{\text{block}}}\sum_{j=1}^{n_{\text{block}}}\left(E_j^{\text{block}} - \langle E\rangle_{\text{block}}\right)^2 . & (12b)\end{aligned}$$

This is the so-called blocking technique [16] to get an estimate for the error bar at the presence of serial correlation between successive samples. Otherwise, evaluating the variance in the straightforward way would provide an underestimated small error bar, due to serial correlation of successive data points, which artificially reduces the variance[4]. Using the blocking technique and given that $\frac{M}{n_{\text{block}}}$ is high enough, there is no serial correlation between the $E_j^{\text{block}}$ values anymore, so that $\sigma$ can be correctly estimated.

Plotting $\sigma_{\text{block}}$ as a function of $n_{\text{block}}$ and assuming that $M$ is sufficiently large, for the correct estimate of the error a plateau is observed. We remark that in general $\langle E\rangle_{\text{block}}$ is not equal to $E$, but as long as $M$ is large enough, each $E_j^{\text{block}}$ will be very close to $E$, so that eventually $E$ agrees with $\langle E\rangle_{\text{block}}$ within one standard deviation.

| $n_{block}$ | $\langle\mathcal{E}\rangle_{\text{block}}$ | $\langle\mathcal{E}_{kin}\rangle_{\text{block}}$ | $\langle\mathcal{E}_{pot}\rangle_{\text{block}}$ |
|---|---|---|---|
| 4 | −2.07 K | 12.20 K | −14.26 K |
| 8 | −12.12 K | 8.21 K | −20.33 K |
| 12 | −1.60 K | 13.89 K | −15.49 K |
| 16 | −2.36 K | 11.57 K | −13.93 K |
| 24 | −2.58 K | 16.18 K | −18.76 K |

Table 2: The mean local energies per particle for the liquid phase of $^3$He with respect to different number of blocks. All results were obtained using $\psi_{\text{FSWF}}$ averaged over $M = 10^8$ sampling points and $N = 66$ .

Looking at Table 2 it is apparent that the FSWF exhibits very large fluctuations in $\langle\mathcal{E}\rangle_{\text{block}}$ for different $n_{\text{block}}$. From this it follows that it is impossible to determine a reliable mean value and an associated error bar, which clearly characterizes the sign problem of the FSWF. Figs. 1 and 2 demonstrate that the sign problem is due to the alternating sign of the weights, since the fluctuations of the local energies are of the same magnitude that we have found using the ASWF.

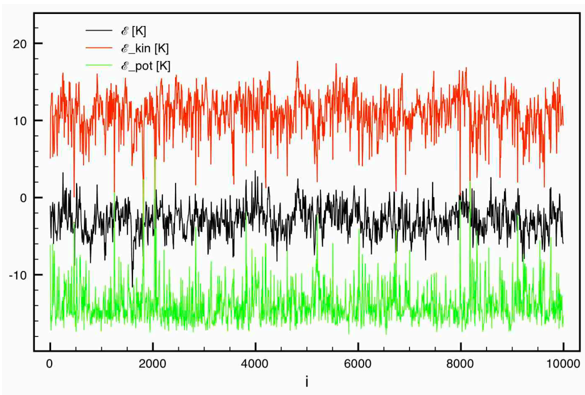


Figure 1: The instantaneous local energies per particle $\mathcal{E}^{loc}$, $\mathcal{E}^{loc}_{kin}$ and $\mathcal{E}^{loc}_{pot}$ for 66 particles of liquid $^3$He using $\psi_{\text{FSWF}}$.

[4]Since the Central Limit Theorem requires independent random samples.

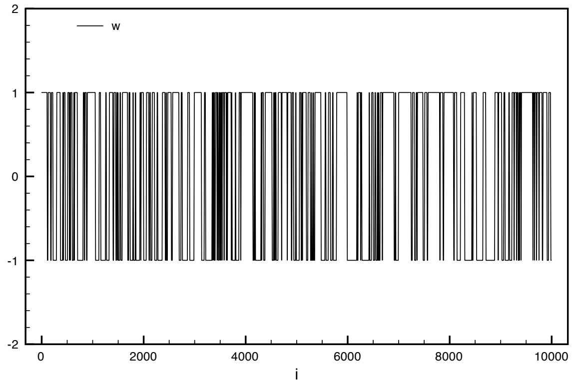


Figure 2: The instantaneous weights $\omega_i$ (see Eq. 9), as obtained using $\psi_{\text{FSWF}}$ for the liquid phase of $^3$He with $N = 66$.

It is important to emphasize, that the sign problem of the FSWF differs from the infamous fermion sign problem of Green's Function [17] or Diffusion Monte Carlo,[18] because in principle it should be possible to find a viable solution to eliminate the former. Nevertheless, the convergence is drastically reduced, so that in many cases (like the one that we have just illustrated) it is practically impossible to get reliable results.

# 3 The Antithetic Shadow Approach

A first attempt [12] to solve the sign problem is to introduce new auxiliary shadows, which will carry the opposite sign with respect to the original ones. The idea is that this will lead to a direct summation of opposite contributions and eventually to a faster convergence. From now on we will indicate the original shadows as $S^+$ and the auxiliary ones as $S^-$.
It can be easily proved that in one dimension

$$\begin{aligned} e^{-c(x-s^+)^2} &= \frac{\sqrt{\sigma_1^2+\sigma_2^2}}{\sqrt{2\pi}\sigma_1\sigma_2}\int ds^-\, e^{-\frac{(x-s^+)^2}{2\sigma_1^2}} \\ &\times\ e^{-\frac{(x-s^-)^2}{2\sigma_1^2}}\, e^{-\frac{(s^++s^--2x)^2}{2\sigma_2^2}}, \end{aligned} \quad (13)$$

where $\sigma_1$ and $\sigma_2$ must satisfy the relationship

$$c = \frac{2\sigma_1^2+\sigma_2^2}{2\sigma_1^2\,(\sigma_1^2+\sigma_2^2)}\,. \quad (14)$$

It is straightforward to adopt this identity within the FSWF, replacing the kernel $\Xi(R, S)$ with [5]

$$\Xi(R, S^+, S^-) = e^{-\sum_{i=1}^{N}\left[\frac{(\mathbf{s}_i^+-\mathbf{r}_i)^2+(\mathbf{s}_i^--\mathbf{r}_i)^2}{2\sigma_1^2}+\frac{(\mathbf{s}_i^++\mathbf{s}_i^--2\mathbf{r}_i)^2}{2\sigma_2^2}\right]}. \quad (15)$$

Setting $\sigma_2 \ll 1$, $S^-$ will be almost exactly opposite to $S^+$ with respect to $R$. We note that for symmetry reasons it is possible to write

$$\begin{aligned} \psi_{\text{FSWF}} &= \psi_p(R)\int dS^+dS^-\,\Xi(R,S^+,S^-) \quad (16) \\ &\times\ \big(\det(\phi_\beta(\mathbf{s}^+{}_\alpha))\,\psi_s(S^+) \quad (17) \\ &+\ \det(\phi_\beta(\mathbf{s}^-{}_\alpha))\,\psi_s(S^-)\big)\,. \end{aligned}$$

In this way, $S^-$ will almost always carry the opposite sign of $S^+$ whenever $R$ will be close to the nodal surface of the SD, which is exactly when the sign problem arises. If this is the case, the sum of two opposite contributions, that explicitly appears in the wave function, will give rise to a much faster convergence of the average. For this reason we will call $S^-$ an antithetic shadow and the corresponding new expression for the FSWF Antithetic Fermionic Shadow Wave Function, denoted as $\psi_{\text{aFSWF}}$.

Using $\psi_{\text{aFSWF}}$, the best results are obtained by sampling from the pdf defined as the absolute value of

$$\begin{aligned} \mathcal{P} &= \psi_p^2(R)\,\Xi(R,S_1^+,S_1^-)\,\Xi(R,S_2^+,S_2^-) \quad (18) \\ &\times\ \big(\det(\phi_\beta(\mathbf{s_1^+}{}_\alpha))\,\psi_s(S_1^+)\ \det(\phi_\beta(\mathbf{s_1^-}{}_\alpha))\,\psi_s(S_1^-)\big) \\ &\times\ \big(\det(\phi_\beta(\mathbf{s_2^+}{}_\alpha))\,\psi_s(S_2^+)\ \det(\phi_\beta(\mathbf{s_2^-}{}_\alpha))\,\psi_s(S_2^-)\big) \end{aligned}$$

and hence

$$\begin{aligned} \omega_i &= \frac{\mathcal{P}}{|\mathcal{P}|}\left(\frac{1}{\det(\phi_\beta(\mathbf{s_1^+}{}_\alpha))\,\psi_s(S_1^+)}\right. \\ &+ \left.\frac{1}{\det(\phi_\beta(\mathbf{s_1^-}{}_\alpha))\,\psi_s(S_1^-)}\right) \\ &\times \left(\frac{1}{\det(\phi_\beta(\mathbf{s_2^+}{}_\alpha))\,\psi_s(S_2^+)}\right. \\ &+ \left.\frac{1}{\det(\phi_\beta(\mathbf{s_2^-}{}_\alpha))\,\psi_s(S_2^-)}\right). \end{aligned} \quad (19)$$

At first sight it might appear that with our antithetic shadow approach substantial progress has been made towards solving the sign problem. Unfortunately, for $\sigma_2 \ll 1$ the Gaussian

$$e^{-\frac{(s^++s^--2x)^2}{2\sigma_2^2}} \quad (20)$$

becomes very narrow and therefore involves large fluctuations in the kinetic energy, that get even more severe as $\sigma_2$ decreases. This behavior is evident by noticing the magnitude of the kinetic energy fluctuations of Fig. 3, in particular when comparing it with Fig. 1.

[5] Normalization factors are always omitted.

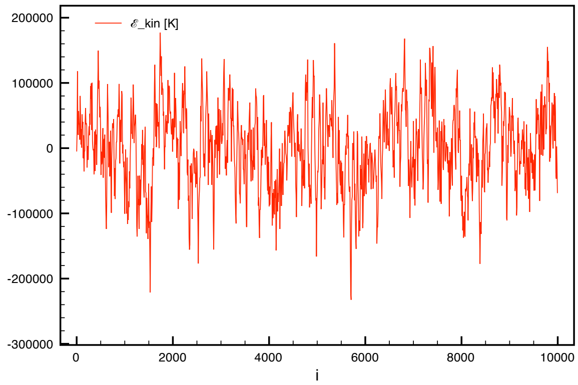


Figure 3: The instantaneous local kinetic energy per particle $\mathcal{E}_{kin}^{loc}$ for 66 particles of $^3$He in the liquid phase using $\psi_{\text{aFSWF}}$ with $\sigma_2 \approx 0.01$ Å.

| $n_{block}$ | $\sigma_2 \approx 0.5$ Å | $\sigma_2 \approx 0.01$ Å | $\sigma_2 \approx 0.001$ Å |
|---|---|---|---|
| 4 | 25.6 K | 1040.5 K | −4688389.6 K |
| 8 | −1.0 K | 899.8 K | −157032.5 K |
| 12 | 118.8 K | 262.2 K | −1501955.0 K |
| 16 | −6.9 K | −851.0 K | −863894.5 K |
| 24 | 1.4 K | −1777.0 K | 13943120.4 K |

Table 3: The mean energy per particle $\langle\mathcal{E}\rangle_{\text{block}}$ of liquid $^3$He. The results were obtained for $N = 66$ by sampling $\psi_{\text{aFSWF}}$ with $M = 10^7$.

Looking at the total energies of Table 3 it may seem that, using the antithetic shadow approach, the results are even worse than before, notably when $\sigma_2$ is small. Nevertheless, the sign problem is indeed substantially reduced as demonstrated by Fig. 4. In fact, the comparison with Fig. 2 clearly exhibits a stabilization of the sign. As a consequence, the evaluation of the potential energy is indeed dramatically improved, as given in Table 4 and in contrast with Fig. 1.

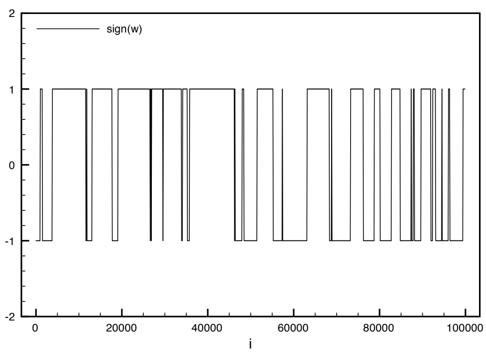


Figure 4: The instantaneous weights $\omega_i$ (see Eq. 19) of liquid $^3$He with $N = 66$ using $\psi_{\text{aFSWF}}$ with $\sigma_2 \approx 0.01$ Å.

| $n_{block}$ | $\sigma_2 \approx 0.5$ Å | $\sigma_2 \approx 0.01$ Å | $\sigma_2 \approx 0.001$ Å |
|---|---|---|---|
| 4 | −16.63 K | −16.12 K | −16.42 K |
| 8 | −15.88 K | −15.91 K | −16.45 K |
| 12 | −16.28 K | −15.94 K | −17.09 K |
| 16 | −16.75 K | −16.12 K | −16.35 K |
| 24 | −15.98 K | −17.20 K | −12.05 K |

Table 4: The mean potential energy per particle $\langle\mathcal{E}_{pot}\rangle_{\text{block}}$ using $\psi_{\text{aFSWF}}$ with $M = 10^7$ and $N = 66$. When $\sigma_2$ becomes too small the results deteriorate because of the increasing autocorrelation between the samplings points.

Even though using the antithetic approach in its current form it is not possible to directly evaluate the energy and optimize $\psi_{\text{aFSWF}}$, it anyhow alleviates the sign problem and allows to reliably evaluate all observables that do not imply any derivatives of the wave function.

Finally, we wish to point out an aspect of our approach that needs to be improved in the future. The pdf of Eq. 19 that we used originates from a simple mathematical manipulation in order to sample from a product rather than a sum of functions, since the latter can not be effectively sampled.[11] However, this entails that the SD may become arbitrarily close to zero and thus the corresponding weights unbounded. The fact that the variance of the weights is therefore infinite necessitates an improved sampling function.

## 4 The Artificial Shadow Correlation Method

As an alternative scheme to solve the sign problem we propose another method, which forces the shadows $S_1$ and $S_2$ to almost overlap so that the product of the two corresponding SD will be always positive. In order to achieve this, we insert the artificial term $e^{-k\sum_{i=1}^{N}(\mathbf{s}_{1\,i}-\mathbf{s}_{2\,i})^2}$, that correlates $S_1$ with $S_2$. We therefore call this technique the artificial shadow correlation method. However, inserting this artificial term into Eq. 7 leads to a systematic bias in the energy due to the non-physical nature of the additional expression, which is only present to avoid the sign problem. Nevertheless, considering the energy per particle $\mathcal{E}(k)$ as a function of the fictitious parameter $k$, it is still possible to estimate the energy. Fitting $\mathcal{E}(k)$ for different $k$ values with an arbitrary function admits to extrapolate to $k = 0$, where the additional term is identical zero and the correct energy $\mathcal{E}(k = 0)$ is recovered. However, as displayed in Fig. 5 the accuracy of the energy estimation crucially depends on the particular function to extrapolate $\mathcal{E}(k)$ to $k = 0$.

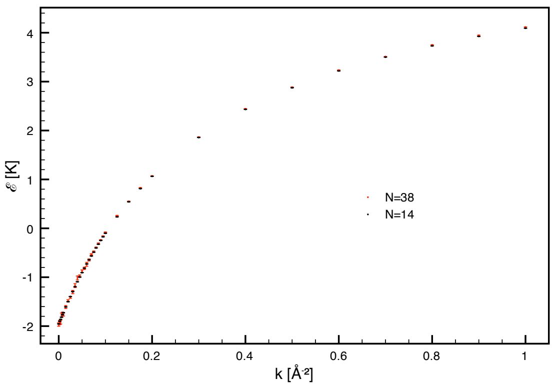


Figure 5: The energy per particle $\mathcal{E}(k)$ with respect to the fictitious parameter $k$.

In order to demonstrate this approach we fit $\mathcal{E}(k)$ using the functions

$$f_2(k) = \frac{A\,k^2 + B\,k + C}{k^2 + D\,k + E}, \tag{21a}$$

as well as

$$f_3(k) = \frac{A\,k^3 + B\,k^2 + C\,k + D}{k^3 + E\,k^2 + F\,k + G}\,. \tag{21b}$$

We find that both functions pass Pearson's chi-square test for both $N = 14$ and $N = 38$. However, we were not able to obtain reliable results for $N = 66$ whenever $k < 0.4$ Å$^{-2}$. That is why in Table 5 only results for $N = 14$ and $N = 38$ with $k > 0.4$ Å$^{-2}$ are reported and compared to the values of plain FSWF calculations. While $f_2(k)$ is not flexible enough to yield satisfactory results, $f_3(k)$ may constitute an improvement. However, due to the large number of fitting parameters that needs to be determined, at this stage the statistical uncertainty is much too high to obtain any meaningful result.

| $N$ | $\mathcal{E}$ | $f_2(k=0)$ | $f_3(k=0)$ |
|---|---|---|---|
| 14 | $-1.9535 \pm 0.0023\,\mathrm{K}$ | $-1.89 \pm 0.19\,\mathrm{K}$ | $-2.0 \pm 3.1\,\mathrm{K}$ |
| 38 | $-1.966 \pm 0.035\,\mathrm{K}$ | $-1.78 \pm 0.11\,\mathrm{K}$ | $-2.2 \pm 2.9\,\mathrm{K}$ |

Table 5: The energy per particle $\mathcal{E}$, as obtained by direct FSWF simulations and by fitting $f_2(k)$ as well $f_3(k)$, where $0.4$ Å$^{-2}$ $< k <$ $100$ Å$^{-2}$, using 25 points each with an error bar of $\sim 10^{-3}$ $K$.

## 5 Conclusions

The extension of the SWF to fermionic systems, which has been outlined here, entails a serious sign problem that makes it impractical - barring additional technical improvements - to simulate the liquid or any other non-crystalline phase of a many particle system. We have presented two novel methods to solve this problem, the antithetic shadow approach and the artificial shadow correlation method. The former is a viable approach to alleviate the sign problem and allows to calculate all expectation values that do not depend on the derivative of the wave function, such as the potential energy. However, it does not permit to calculate the kinetic energy and therefore in particular not the total energy. Nevertheless, our second method may represent an interesting avenue to facilitate exactly that and eventually solve the sign problem. Unfortunately, in its present form the extrapolation to $k = 0$ is simply not accurate enough.

Further advances that we are currently investigating, as well as a conclusive study on liquid $^3$He will be presented elsewhere.

## 6 Acknowledgments

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# Open Questions

## Which New Prospects for an Efficient Prevention and Treatment of Cardiovascular Diseases could be Gained by a Systemic Examination of the Cardiovascular System?

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## 1 Cardiovascular diseases are a disaster of the XXI century

The cardiovascular system (CVS) is an essential component in human health, as the background level of functioning of nearly all organs and systems depends on the blood supply level. It is of a very complicated dynamic mechanism by a type of the closed system of connecting vessels with variable parameters in all its structural segments - heart, vascular walls, as well as intravascular fluid – blood. The system is analogous to water, although almost all its values are variable, from parameters of the pump function (heart) to values of unstable vascular calibers, blood pressure, linear and volumetric velocities, transverse and longitudinal intravascular hydrodynamic pressure depending on the load of the vascular "hemo-supply".

Cardiovascular diseases are an urgent medical and social problem nowadays because of high rates of morbidity, mortality, and disability, indicating the low efficiency of applied methods for vascular diagnosis and treatment.

Today, occupying first place by spreading, cardiovascular diseases cause more than half of all deaths and one third of disability, mainly due to uncompensated cardiovascular conditions - heart attacks and strokes (according to statistics from WHO and Ministry of Health of Ukraine).

3/4 of the population is suffering from cardiovascular pathologies in Ukraine alone and it causes death in 62.5% cases; that is much higher than in developed countries. Recently, the spreading of ischemic heart diseases has increased in Ukraine from 10 000 to more than 20 000 per 100 000 of the population. And more than 5 million patients with hypertonic disease are registered in Ukraine.

## 2 Multi-problems concerning diagnosis and treatment

Despite of considerable efforts of scientists, there is no tendency to decreasing of morbidity and mortality indexes of cardiovascular diseases (CVDs) today. In fact, the world has not enough efficient technologies for preventive examination of the cardiovascular system. They must not be for palliative adaptation to the sickly state, but for restoration of the system to the level of autoregulation and self-control. Some important factors have not been included in basic and applied research. Let us name the most important:

1. **Static examinations predominate.** Local CVS examination does not consider interconnections between dynamics of segments and general dynamics of the vascular system on various regional levels. Thus the corresponding treatment has only palliative nature and is not directed to needs of the initial and secondary prevention of cardiovascular diseases.

2. **There is no systemic approach to the examination of CVS as an entire system of vascular "hemo-supply" with multiple intersystem connections.** A role of arterial and venous dampers is ignored for blood redistribution in various regional reservoirs.

3. **There is no systemic approach, when the organism is considered to be a controlled system,** to peculiar features of hydrohemodynamic laws in vivo for providing functioning of interdependent segments of the closed CVS: heart - major arteries - peripheral arteries – arterioles – capillaries – venules – peripheral veins – major veins - heart. That is why the one-moment examination of CVS requires quite new technological approaches with detection of polyvector characteristics of all levels and concretization of

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an injured area and influence of the area on functioning of the whole system.

4. **The venous system is not examined enough** as it is considered to be in a shadow and less accessible for life-time functional examination
5. **There is a lack of profound examinations of correlation of hemodynamic characteristics of major and peripheral arteries, veins and capillaries for providing coordinated CVS functioning**
6. **Current diagnostic and treatment measures are not sensitive enough for early disorders in CVS functioning.**
7. **One-sided CVS examination.** There is a gap between local medical examination and a global approach under mathematical modeling of CVS according to cybernetics because of the lack of local indicators for the vascular system condition. One cannot make global conclusions about the functioning of the entire system by one CVS parameter. Such an approach to the CVS investigation is too expensive, thus causing "rejuvenation" and progression of CVDs. When we analyzed the CVD statistics in Ukraine, Europe, and the world, we observed the following tendency – 20 years ago people older than 40-50 years had CVDs, while today the age is older than 30 years. There are rare cases of stroke among teenagers and even sudden death during physical lessons in schools, which had never been observed before
8. **Lack of a single approach in vivo to blood as a biological and biochemical non-Newton liquid** causes physicians to be mistaken about the properties of blood – it is perceived as an ordinary liquid.
9. **Usage of absolute values** as a statement of incorrect functioning of the system not taking into account parameters of reactivity and adaptation of CVS in conditions of disorder of internal homeostasis and changes of environmental parameters (meteorological factors), neglecting integral parameters when estimating CVS functioning causes a principally wrong static (but not dynamic) approach in analyzing the functioning of the dynamic blood circulation system.
10. **Lack of profound examinations of correlation between immunodeficiency states** and development of any vascular pathology causes accompanying conditions for progression and spreading of cardiovascular diseases.

# 3 Conclusion

The current level of examination of the cardiovascular system requires new analytical approaches to processing of various vector characteristics of all local segments and regional levels of the CVS with concretization on the injured area and local influence of the area on the functioning of the entire system. Any treatment course ultimately requires a CVS monitoring to analyze hemodynamic changes of adaptive or pathological reorganization in the vascular bed. We invite everyone concerned to participate in the discussion of the above mentioned problems. And we gladly will keep up the discussion.

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# What Is the Role of Epidemiological Factors in Shaping the Social Imperative of Monogamy

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## 1 Introduction

”That for which nearly a year had been Vrosnky’s sole and exclusive desire , supplanting all his former desire: That for which Anna had been impossible, dreadful, but all the more betwiching dream of happiness, had come to pass. Pale, with trembling lower jaw, he stood over her, entreating her to be calm, himself not knowing how nor why. ... ‘It’s all over´, she said. ‘I have nothing but you left. Remember that.´“[1]

Anna Karenina is one of the most prominent and at the same time most tragic adulterers in world literature. What begins as passionate but forbidden love between her and Alexey Vronsky leads to years of ostracism and finally reaches its climax in Anna Karenina’s suicide. In the above scene, where the sexual aspect of their relationship cannot be overlooked, Anna Karenina already foretells her fate: ”It’s all over“.

The novel is a grand example of how individuals are torn apart between the social imperative of monogamy and their intrinsic passions. Monogamy is indeed a puzzling social construct, since there seem to be two incompatible souls in us: Our wish for intimacy, consistency, and security on the one hand and our adventurous desires on the other. Some scientists interpret these two souls in a way that suggests that our own evolutionary biology is in conflict with norms and imperatives imposed on us by society and culture.

It seems difficult, if not impossible, to determine what is the homo sapien’s ”natural“ way of living: Monogamic, polygamic, or even promiscuous. An easier task is to point to historical and evolutionary facts that may have led to the sexual norms dominating our society.

Reasons for a monogamous lifestyle are manifold. The upbringing of a human child is laborious, therefore both father and mother are involved. By simple evolutionary arguments, the parents want to make sure they don’t raise other peoples’ children. Economic factors as well as ancient religious commandments play a role for the appearance of monogamy as the primary form of family organization in the western world. These have been discussed elsewhere, but we think that one crucial aspect is missing from the discussion on monogamy.

An eye-catching reason for a monogamous lifestyle is that, medically speaking, it makes sense. Staying with one lifelong sexual partner minimizes the risk of falling ill with a sexually transmitted disease (STD) like syphilis, gonorrhea, the human immunodeficiency virus, the human papilloma virus, etc.

Thus, could it be the case that infectiological and epidemiological factors have contributed to the cultural imperative of monogamy? And if yes, in which way and to what extent?

We approach this problem from two perspectives: First, we take on a purely biological view of sexually transmitted diseases and monogamy. In the second part, we try to discuss how our image of monogamy could have been shaped historically by epidemiological factors.

## 2 Do sexually transmitted diseases support the evolution of monogamy from a biological point of view?

From an evolutionary point of view we have to ask the question, if our genetic constitution could have been shaped by sexually transmitted diseases and if human behaviour can be determined by our genes. A genetic determination of our lifestyle cannot be ruled out easily, but reducing the complexity of an individual’s behaviour to just a few genetic factors falls short of taking life events, education, and development of a person into consideration.

A possible way, in which sexually transmitted diseases could have led to a monogamous lifestyle by natural selection, though, is an actual decrease in an individual’s fertility rate due to the STD. In this way, monogamous behaviour could be imprinted in our genetic material.

An STD can lead to a decreased fertility rate by different mechanisms: Death of a patient of reproductive age, impairment of the reproductive system, external mutilations that make the patient less attractive during the reproductive age span, or serious affection of the child during pregnancy or birth leading to death or decreased fertility rate of the child.

Since there are many STDs, this will be discussed using the example of syphilis. Syphilis was first described in the late 15th century when it began to spread in the mediterranean area, especially in Spanish an Italian port cities before it became epidemic for the next 50 years all over Europe. Syphillis does not kill the patient during the reproductive

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age – patients might die due to complications like syphilitic aortitis but this normally occurs only decades after the primary infection. Syphilis usually does not impair the reproductive system of men, but in women it is associated with increased rates of abortion and fetal death. Children whose mothers are infected might suffer from congenital syphilis since infection can occur during pregnancy or birth but not all of the children will be affected by congenital syphilis. Primary syphilis only causes a small, indolent lesion at the site of infection, so that the infection can only be recognized by potential partners by examination of the genitals. Secondary syphilis can cause a rash that usually disappears quite soon. There are long latencies, so that usually the promiscuous behavior is not impaired in these states of the disease. Tertiary syphilis may cause the so called gummata, soft subcutaneus tumors that may be a few centimeters in diameter, and by this cause severe mutilation of the patient. These mutilations might decrease the fertility rate of the patient since they are easy to identify by potential partners. By these mechanisms syphilis might lead to a decreased fertility rate, but most severe symptoms occur years to decades after the primary infection, so that there is enough time to produce children.[2,3]

All in all, the fertility rate of promiscuous people can be decreased due to syphilis but it remains unclear whether the possibility to produce more children due to in increased number of partners outweighs the negative effects of a probably only mildly decreased fertility rate after the infection. Valid statistic data regarding this topic would be necessary to solve this question.

In our opinion, monogamic behavior cannot be explained by a purely biological evolutionary process.

## 3 A sensation of danger: Epidemiological factors from a historic point of view

There is another way in which the social imperative of monogamy could have been shaped by epidemiological factors. Historically, the real statistical threat of an STD does not play nearly as big as a role as the sensation of danger that it causes. The way in which the danger of the disease is perceived and interpreted in a society has influence on an individual's sexual life.

Again, the syphilis epidemic [3] of the late 15th century is discussed as an example. There are diverging opinions about how syphilis arrived in Europe. Some argue it arrived with the return of the Columbus expedition, others argue that it had existed in Europe before 1492. It was soon clear, though, that this novel disease was transmitted by sexual contact and as soon as it was associated with sexual intercourse it became associated with the female body. Men were mostly considered victims of the disease while the woman's womb was held responsible for transmitting syphilis.[4] One theory for the emergence of syphilis, first described in 1615 by Giovanni Tomasso Minadoi in Padua, embraced that virulent material resulted when the semen of different men is mixed in a woman's uterus.[5] This medical explanation on how men could get infected with the disease obviously dovetails with two imperatives: Women should should engage in an absolutely monogamous lifestyle, and men should avoid sexual intercourse with women likely to sleep with more than one man, i. e. prostitutes.

Indeed, one can state that the perception of prostitution changed because of the syphilis epidemic in the 15th century. Prostitution had always been linked to disease but in the Renaissance it was viewed quite positively, because it was not only about sex and money. Guido Ruggiero argues that prostitution in the Renaissance was "as much about buying love and falling in love as about sex."[6] While a beautiful young wife offered security and reputation to a man, courtesans offered sex and love. Thus, it is not surprising that brothels were often publicly run and placed in the center of the cities, visible for everyone.

But as early as 1546, Henry VIII closed public brothels and Scottish edicts banned prostitutes in 1560 due to their connection with the new disease. And although prostitution did not get eradicated by these efforts, its social acceptance declined.

The discourse on monogamy was certainly shaped by the syphilis epidemics, and not only by syphilis. Looking at more recent developments, the discourse on the human immunodeficiency virus would also serve as a splendid example of how the sensation of danger influences an individual's sexual behaviour.

## 4 Conclusion

It is not likely that sexually transmitted diseases have led to monogamic behaviour by imprinting them into our genetic make-up in the process of natural selection. We argue, though, that epidemiological factors probably have contributed to our ideals of monogamy via the sensation of danger that sexually transmitted diseases cause in a society. In this context one arrives at a related questions: How much overlap is there between the actual, statistical threat of a sexually transmitted disease and the peoples' fear of it? And in which way is the sensation of danger related to the actual threat?

As a conclusion, we would like to pose the question if these two views, the biological or medical view and the historic or sociological view on the epidemiology of sexually transmitted diseases, can even be separated cleanly. Certainly, the distinction we make between "biology" and "history", between how monogamy was shaped by "nature" or by "culture", is not nearly as unambiguous as we present it in this article.

Unquestionably, sexually transmitted diseases do not play any role in Anna Karenina's or Alexey Vronsky's thoughts. The most present threat for them is loss of reputation and

[3] In the late 15th century there was no distinction between a plethora of sexually transmitted diseases that early modern doctors subsumed under the term "The Veneral Disease"

exclusion from society. This eventually leads to Anna Karenina's suicide, one of the most tragic moments in world literature. We conclude that no matter how the imperative of monogamy was shaped it undoubtedly provides some of the most splendid material for reading enjoyment.

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# Is Computer Go Solvable?

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## 1 Introduction

Go ('weiqi' in Chinese and 'igo' in Japanese) [1] is an ancient board game originating from China that has been widely played in East Asia. Nowadays Go is being more and more popular throughout the world. In contrast to many other strategic games, including chess, that have been conquered by modern computers many years ago, Go remains a formidable challenge to artificial intelligence [2] due to the enormous branching factors of the game tree and, perhaps more importantly, the lack of proper evaluation criteria. The past two decades have seen significant progress in the field of computer Go, in which the level of computer players was promoted from that of human beginners to reasonable amateurs. However, there is still a long way to go in order to achieve the following two goals: 1) to reach the level of the best human players, 2) to resolve Go completely, i.e. to find the best possible next moves. Although not an expert in the field of computer Go, I will first summarize succinctly in this letter the basic aspects of Go and computer Go and then discuss possible strategies for future development of computer Go from the perspective of a human player.

## 2 Basics and challenges for computer Go

Go is played by two players, viz, the black side and white side on a 19 by 19 board. The game starts with an empty board and the two players then place the black and white stones alternatively on the vacant intersections of the grid. There are only two basic rules. First, a stone or a cluster of stones is 'captured' and should be removed from the board when entirely surrounded by enemy stones. For example, in Figure 1 the two black stones are 'captured' and should be taken away when white places another stone at point A. Second, the same pattern is not allowed to appear in two consecutive moves in order to prevent trivial unending cycles in a game. For example, in Figure 2, white cannot place a stone in the place of the captured stone immediately after black plays a move at point A.

The large size of the board together with the simplicity of the rules renders most of the moves 'in principle possible' and consequently leads to huge branching factors of the game tree. Therefore, the first major difficulty is that it is virtually impossible for modern computers to exhaust all possible games when looking for the best next moves. Putting aside a complete Go game, the 'life and death' problem in Go is already proved to be NP-hard [3,4] and the endgame is proved PSPACE-hard. Therefore, it is necessary to introduce effective evaluation rules for a given pattern in order to judge the efficacy of a certain set of moves without finishing the game in the calculation. Here comes the second principle difficulty that is elaborated below.

The basic scoring rule in Go is that the winner has more territory in control. For example, in Figure 3, the white side is the winner because it obviously controls much more than half of the total board, although black captures much more enemy stones. This scoring rule actually imposes difficulties in quantifying simple evaluation rules for the computers. In contradictory to intuition, in many cases the more stones one captures, the worse the situation becomes. Furthermore, in order to evaluate a certain local variant, one has to consider both the local benefits and the effects on other

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parts of the board. The situation can be dramatic. A classical example is shown at the left-below corner of Figure 4. At first sight, it is a disaster for the white side as six white stones (1, 7, 9, 11, 19, 21) are captured and the black side occupies the entire corner. However, the white 'wall' is so influential to the rest of the board that the white is actually far ahead. It should be emphasized that although humans can 'feel' the strength of such a 'wall', it is rather difficult to make the computer 'realize' this in a quantitative manner.

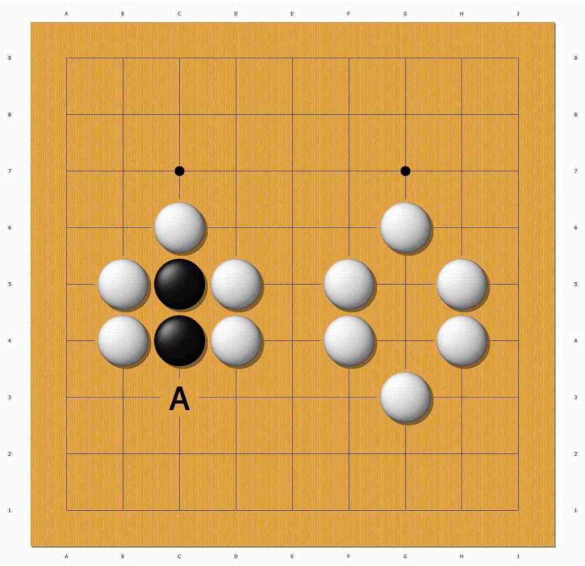


Figure 1: The two black stones are captured when white plays at point A. The captured stones are removed from the board.

# 3 Progress and unsolved problems in the field of computer Go

The first computer Go program dated long back to 1968.[5] However, traditional bruteforce algorithms based on minimax tree search fail largely for computer Go in spite of their prominent success for computer chess. The minimax tree search schemes try to exhaust all possible variants after a certain number of moves, e.g., 50 moves from now, and then choose the best next move by evaluating the patterns obtained after these moves. Due to the huge number of possibilites and the lack of proper evaluation functions, programs were often stuck or made unfavorable judgements. Other strategies were introduced, such as knowledge-based systems to use the available games to facilitate the search and judgements. In general, the level of computer players remained below the human beginner's level until the recent major breakthrough was achieved using Monte Carlo sampling.[6,7]
In Monte Carlo based methods, the computer generates a number of possible next moves and then for each of them tries out randomly a certain number of complete games. The move leading to the best group of hypothetical games is then adopted. The Monte Carlo based strategy circumvents the problem of finding proper evaluation functions by playing out complete games while it tries out as many variants as possible and then leaves the final decision to statistics instead of trying to exhaust all possibilities. Therefore, the Monte Carlo method is much more practical. The level of best computer players was quickly promoted to professional level for 9 by 9 mini-board and reasonable amateur level for the standard 19 by 19 board.

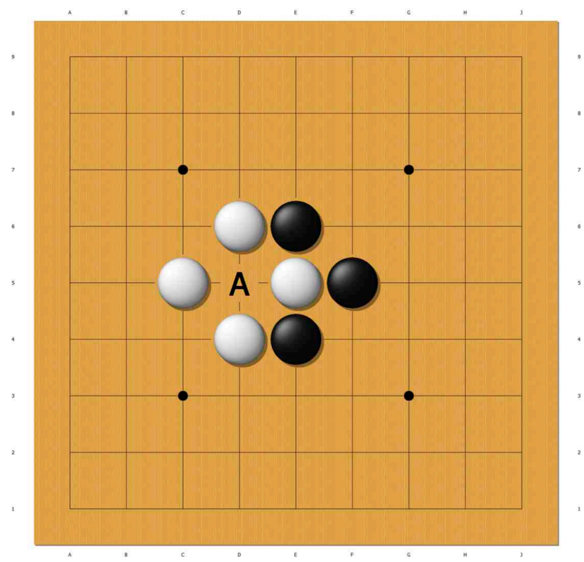


Figure 2: A classical pattern named 'ko' in Japanese and 'jie' in Chinese. When black plays at point A to capture the white stone at the coordinate E5, white cannot place a stone at E5 immediately after that.

In view of the significant progress in computer Go algorithms together with the fast development of computer parallelization, one may expect that the computer Go players will be able to challenge top human players in the near future. However, it should be noted that the Monte Carlo method still has fundamental drawbacks. First and perhaps most important, Go is not really statistical. There is often one single best choice of sequential moves. Meanwhile, some wrong moves can lead to disasters rather than small negative effects. Therefore, a statistical average does not always make sense and the best move is still guaranteed only when exhausting all possibilities. Second, the use of proper evaluation functions is still preferred since playing out complete games is very costly and limits the number of variants that can be tried out.

# 4 Discussions and outlook

As the readers may notice, we came back to the formidable tasks of exhausting the game tree as well as finding proper evaluation functions when analyzing the drawbacks of Monte Carlo sampling, which seem to be unavoidable obstacles in computer Go from a purely mathematical point of view. Instead of continuing thinking about computer algo-

rithms, we classify Go problems into two categories below from the perspective of human players:
1) Specific Go problems that are precisely solvable for human players. The major advantage of modern computers over the human brain is perhaps the speed of calculations. A second advantage is that modern computers have definitely precise memories while even top human players can forget things, as all humans do. Therefore, when a specific Go problem can be resolved by human players in a definite manner during a game or during studies after the game, e.g., many 'life and death' problems as well as 'endgame' problems, there is no reason why computers cannot. Therefore, the NP-hardness of 'life and death' problems as well as unsolvable appearance of many other Go problems of this category are artifacts due to the use of bruteforce strategies. It will be helpful to seek for 'human guidance' in solving these problems when human players know precisely how to do it, namely, the computer Go developers may interact deeply with (strong) human Go players to learn precisely how they tackle these problems and then translate the understanding to the computer. For example, it will be useful to create a filter that reduces the 'possible' moves from the beginning, as human players never scan all the 'in principle possible' moves. Computers may first learn the 'wise' way of thinking and after that use their 'gifted' bruteforce in selected occasions.

2) Rather general problems to which human players apply their 'feelings'. Such problems occur when the player needs to decide the 'flow' of the game without quantified information. I show a simple example in the left-up and right-down corners of Table 4. Human may easily have the visual 'feeling' that the pattern in the left-up corner has more potential than the one at the right-down corner but it is less straightforward to quantify this to the computer. This is a over-simplified question with a more or less definite answer and can be implemented by using an 'influential line'. However, there are many occasions when even top human players may disagree with each other. Human guidance can thus only give qualitative solutions to this problem.

Let us note that it is not necessary to fully resolve the second set of problems in order to challenge human players, to fulfill the goal 1) in the introduction. Therefore, in the near future, the practical strategy might be to work on quantitative (or definite) solutions of Go problems of the first category with qualitative solutions for problems of the second type (or even human control as an intermediate state of development).

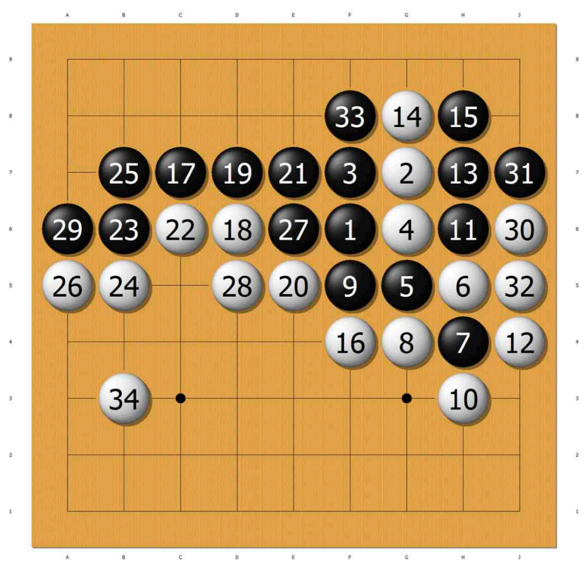

Figure 3: A sample game in a 9 by 9 mini-board. White is the winner since it controls much more than half of the board. Please note that black captures three white stones (2, 4, 14) while white captures only one black stone (7).

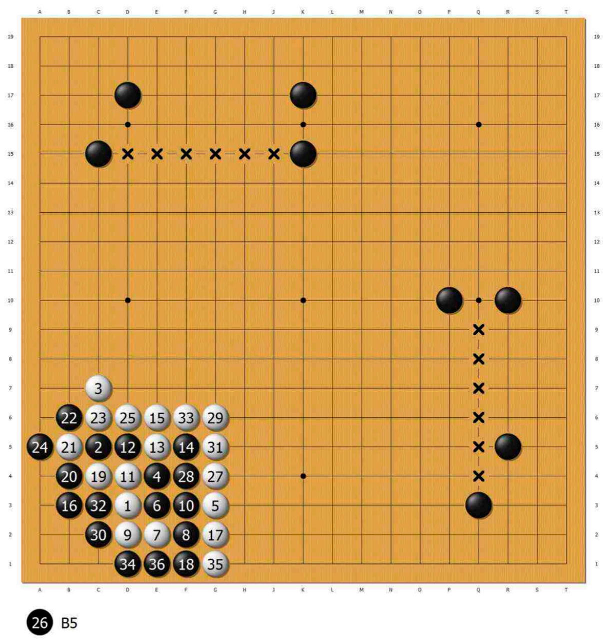


Figure 4: At the left-down corner there is a dramatic variant in which black captures six white stones (1, 7, 9, 11, 19, 21), but is close to be defeated. Note that 26 is at the same position as 21. At the right-down and left-up corners there are two closely-related patterns. Human players can recognize visually that the left-up pattern has more potential than the right-down one.

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# Do Female Bonobos Fake Orgasm?

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## 1 Introduction

Theory of mind (ToM) is the ability to attribute mental states—beliefs, intents, desires, pretending, knowledge, etc.—to oneself and others, and to understand that others have beliefs, desires, and intentions that are different from one's own.[1] There is controversy over the question whether animals other than humans have a ToM. The question is important when assessing the status of humans within the animal kingdom. The social tool of faked orgasm seems to be unique to human beings and thus it is a strong test for the demarcation of human versus animal. Faked orgasm thus provides a novel test of ToM in non-humans. Bonobos are enthusiastic performers of both sexual and deceptive acts and therefore are good subjects for the proposed study.

## 2 Premises and Proposition

Our argument is constructed like an old-fashioned polysyllogism, complete with climax.

### 2.1 Human Females Fake Orgasm

It is a widely known fact that human females can fake orgasm. Indeed, faking orgasm is more common, also among human males, than previously thought.[2] The motives and functions of faking orgasm vary considerably. A person may fake orgasm in order to protect or boost the sensitive egos of their partners; to mask their own insecurity and fear of intimacy; to terminate overlong sexual intercourse; or to enhance their own sexual experience. Some of us may even have witnessed this phenomenon as a participating observer.

### 2.2 Female Bonobos Experience Orgasm

Primates experience something similar to orgasm.[3] For female bonobos the matter is straightforward—they do experience orgasm.[4]

### 2.3 Bonobos Deceive

Many animals deceive animals of their own (intraspecific deception, e.g., foraging deception) and other species (interspecific deception, e.g., mimicry).[5] Primates, and prominently bonobos, do deceive each other.[6] Faking (or pretending) is a special form of deception, a form of Machiavellian intelligence.

### 2.4 Female Bonobos Fake Orgasm

Putting the above (2.1, 2.2 and 2.3) together, we pose the proposition (or hypothesis) that female bonobos can fake orgasm. And, appealing to probability, if they can they surely will.

## 3 Method and Apparatus

The hypothesis formulated in 2.4 can be tested by measuring the behavioural signs ('climax face', vocalizations) and the physiological correlates (increased blood pressure, heart rate, breathing rate, skin conductance; rhythmic pelvic and vaginal contractions) characteristic of true female bonobo orgasms and contrast them with potentially faked orgasms. Evidence will consist of discrepancies between these behavioural signs and the physiological correlates. The hypothesis can be tested using apparatus similar to that for studying human orgasm. Calibration can be done using

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masturbating female bonobos. Apart from enjoying frequent hetero- and homosexual intercourse, bonobos are also keen masturbators. As there is no partner, there is no motivation to fake while masturbating, and a behavioural and physiological profile of true orgasms can be obtained.

# 4 Discussion and Predictions

Sexual behaviour of humans and other animals is fraught with deception and manipulation. Female Indian langurs bob and weave in a typical estrous manner (pseudoestrous solicitation), faking their receptivity, copulating their way into the favour of an infanticidal male.[7] There is also a surprising piscine precedent of non-human faked orgasm: female brown trout (Salmo trutta) can perform a 'false orgasm'.[8] Given the validity of 2.1 – 2.3, the interest in ToM, and the relative ease in conducting the study, 2.4 concerning the presence of faked orgasms in bonobos will probably be confirmed within the next 5 years. Lacking eligible bonobos, we can only submit the hypothesis, but not conduct the necessary tests. Nevertheless, when other scientists succeed in proving faked orgasm in female bonobos, this result will have a major impact on our understanding of primate consciousness and ToM (and we will be happy to share the honours when they are awarded). The proposed research will raise many new questions, one of which challenges males everywhere: Can male bonobos distinguish between real and faked orgasms of their female partners, and if they cannot, do they have a partial ToM deficit?

# 5 Acknowledgement

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