Quantum Monte Carlo in the Apuan Alps IX



International Workshop Saturday 26th July - Saturday 2nd August 2014 The Apuan Alps Centre for Physics @ TTI, Vallico Sotto, Tuscany, Italy

vallico.net/tti/tti.html and vallico.net/casinoqmc/

This is the programme document for the 2014 international workshop 'Quantum Monte Carlo in the Apuan Alps' the ninth such event to be held in Vallico Sotto. The general purpose of workshops at this venue is to *gather together limited numbers of able scientists to discuss topics of mutual interest in greater depth than is normally possible* (the original motivation for the well-known Solvay meetings in the 1920s, but this time for people without Nobel prizes); in that sense TTI – run on the smallest of shoestring budgets – has been described as an 'Erice for peasants'.

The focus of the current meeting will be on the quantum Monte Carlo (QMC) method and related techniques in computational electronic structure theory, and their use in understanding the quantum-mechanical behaviour of atoms, molecules, and condensed matter. For many types of problem the accuracy of quantum Monte Carlo is much better than that of the more widely-used density functional theory, and its scaling with number of atoms is much more favourable than that of high-level quantum chemistry. Unlike most other methods, it is also fully capable of exploiting the full power of the largest computers in the world (the Cambridge CASINO QMC code, for example, has been shown to run efficiently on over half a million cores). All topics related to applications of QMC and/or theory and algorithm development will be welcome, though it is expected that broader topics in the general area will also be discussed.

A particular topic of interest is the relationship between QMC and density functional theory. In particular, we hope to look towards obtaining a better understanding of the relative benefits of QMC/DFT in systems and situations where DFT often fails, such as in weakly-interacting systems, strongly-correlated materials, metal-insulator transitions, magnetic properties, and biological systems. Furthermore, it is intended to look into the better integration of DFT and QMC codes. In industrial applications, where users typically require ease-of-use and a graphical user interface, how can we move towards a situation where the user may do e.g. pre-screening of candidate structures with the faster DFT, then press a 'Make the Answer Better button' which feeds the relevant wave function files into a QMC programme and spits out reliably accurate energetics for the selected problems? It is also if interest to understand how to 'move the atoms' in QMC, that is, how to exploit the power of QMC in cheaper DFT and classical-force-field molecular dynamics calculations (in the context of 'embedding methods' or otherwise). Additionally we can look at how to use QMC to develop better exchange-correlation functionals for use in DFT. We therefore warmly encourage the participation of DFT people who may never have a run a QMC simulation in their lives but are nevertheless interested in the topic. Suggestions for alternative discussion topics and other proposals are welcome.

The format of TTI workshops is intended to encourage a relaxed and intellectually-stimulating atmosphere rather different to the usual 8am to 7pm grind of your regular conference. Formal talks are restricted to the mornings, and participants are given the freedom and space to think and to contemplate and discuss the issues at hand. Healthy recreational activities such as mountain walks are to be organized in the afternoons, and it is hoped that by taking part in these whilst breathing the clean air of the Apuan Alps and sampling local Tuscan food, the participant will be able to return home mentally and physically refreshed as well as having deepened their understanding of science.

1 LIST OF REGISTERED PARTICIPANTS

Dario Alfè UCL, London, U.K. d.alfe at ucl.ac.uk Sam Azadi Imperial College, London, U.K. s.azadi at imperial.ac.uk Giovanni Bachelet Sapienza University, Rome, Italy giovanni.bachelet at roma1.infn.it Dario Bressanini Università dell'Insubria, Italy dario.bressanini at uninsubria.it chushb09 at lzu.edu.cn Shibing Chu Lanzhou University, China Ron Cohen University College, London, U.K. ronald.cohen at ucl.ac.uk Gareth Conduit University of Cambridge, U.K. gjc29 at cam.ac.uk Csaba Daday University of Twente, Holland dadaycs at gmail.com Caterina De Franco University of L'Aquila, Italy caterinadefranco at gmail.com Andrea Droghetti Trinity College, Dublin, Ireland drogheta at tcd.ie University of Torino, Italy Roberto Dovesi roberto.dovesi at unito.it Lancaster University, U.K. Neil Drummond n.drummond at lancaster.ac.uk Edgar Engel University of Cambridge, U.K. eae32 at cam.ac.uk Matthew Foulkes Imperial College, London, U.K. wmc.foulkes at imperial.ac.uk Leonardo Guidoni University of L'Aquila, Italy 1.guidoni at gmail.com Nic Harrison Imperial College, London, U.K. nicholas.harrison at imperial.ac.uk Kenta Hongo JAIST, Japan kenta_hongo at mac.com Blazej Jaworowski Wroclaw University of Technology, Poland jmvarelse at gmail.com Martin Korth University of Ulm, Germany martin.korth at uni-ulm.de Jonathan Lloyd-Williams University of Cambridge, U.K. jhl50 at cam.ac.uk Pierre-Francois Loos Australian National University loos at rsc.anu.edu.au Pablo López Ríos University of Cambridge, U.K. pl275 at cam.ac.uk Ryo Maezono JAIST, Japan rmaezono at mac.com Fionn Malone Imperial College, London f.malone13 at imperial.ac.uk Mariapia Marchi ESTECO S.p.A., Trieste, Italy marchi at esteco.com Bartomeu Monserrat-Sanchez University of Cambridge, U.K. bm418 at cam.ac.uk Elaheh Mostaani University of Lancaster, U.K. emostaani at gmail.com Richard Needs University of Cambridge, U.K. rn11 at cam.ac.uk Carlo Pierleoni University of L'Aquila, Italy carlo.pierleoni at aquila.infn.it Tom Poole Imperial College, London, U.K. thomas.poole10 at imperial.ac.uk James Shepherd Rice University, U.S.A. jjs6 at rice.edu Sandro Sorella SISSA, Trieste, Italy sorella at sissa.it James Spencer Imperial College, U.K. i.spencer at imperial.ac.uk Alex Thom University of Cambridge, U.K. ajwt3 at cam.ac.uk Mike Towler University of Cambridge/UCL, U.K. mdt26 at cam.ac.uk John Trail University of Cambridge, U.K. jrt32 at cam.ac.uk Cornell University, U.S.A. cyrusumrigar at gmail.com Cyrus Umrigar Tack Uyeda JAIST, Japan tueeeda at jaist.ac.jp Will Vigor w.vigor11 at imperial.ac.uk Imperial College, London, U.K. Ching-Ming Wei Academia Sinica, Taiwan cmw at phys.sinica.edu.tw

FAMILY MEMBERS

Kyra Umrigar (16), Jasmine Umrigar (13)

STAFF

Samantha Keil, Saska Towler, Jamie Towler, Lisa Johnson-Davies, Alex Haider

2 FLIGHTS AND TRANSPORT

In this section we explain how to get to the Institute for people flying into our recommended airport - Galileo Galilei Airport, Pisa. It is also possible to fly to Florence (Firenze) which is only slightly further away, though flights to this airport are limited. In principle one could also fly to other airports such as Perugia, Bologna, Ancona, Parma, Milano, Verona, Genova or Roma but you should count on a train ride of up to four or five hours to get to the Institute (we can arrange this for you). A list of airlines flying to Pisa with links is given on the TTI web page (see 'Flying to Italy' in the left-hand column) and there is a map on the Pisa airport web page (http://www.pisa-airport.com/index.php?

lang=_en - click the 'Destinations' link). Americans should note that Delta Airlines operate a direct service to Pisa from New York (the only direct service from outside Europe). Further details about transport, including how to drive to the Institute, are also given on the TTI web site.

Participants should aim to arrive at Pisa airport on Saturday 26th July (Cambridge people are encouraged to come on Friday 25th to help with setting up the venue). If this is not possible - perhaps if flights from your country are irregular - then we recommend having a brief holiday in Florence or elsewhere before coming to TTI, or you could always volunteer to arrive early and be put to work! Please note that late departures are not encouraged because of the summer school taking place immediately after the workshop (in addition to transporting people to airports and so on we need to reboot the entire village and clean everything in less than a day).

How to get to TTI from Pisa airport on Saturday 26th July:

Go to Pisa Centrale train station. To get there from the airport we normally recommend you take a taxi - you can see the taxi rank as soon as you exit the airport terminal building. The *stazione* (phonetic: 'statsionay ferrovia') is a 5-minute journey. However a new and much improved bus service has just been introduced which is much cheaper (1 EUR 30) and leaves every ten minutes (the bus stop is on the left as you walk out of the terminal building - look for the white tent-like structure with 'PisaMover' on the side). Tickets for the bus are available from the Pisamover kiosk in the terminal building (they will also sell you your train ticket..). This is a new service introduced because they've just dug up the railway connecting the airport to the train station in order to replace it with some kind of fancy monorail - see the video here:

http://www.pisa-airport.com/index.php?lang=_en&id_sect=438

Once at Pisa Centrale station you then need to get a train to Barga-Gallicano. This is an isolated station north of the city of Lucca somewhere along a branch line going up the Serchio river valley into the mountains (see the map on the TTI web site). Depending on the train time, you may need to change at Lucca to get the train north. The train will usually be flagged as going to one of four final destinations. "Aulla-Lunigiana", "Minucciano", "Piazza al Serchio" or "Fivizzano". See the printed timetables on the station wall to check where each train stops (for the usual stopping trains Barga-Gallicano is the eighth station stop after leaving Lucca; start getting ready to leave the train after Fornaci di Barga station). The electronic screens in the station show the departure platform ('binario'). Note that in Italian, Departures is 'Partenze', and Arrivals is 'Arrivi' - make sure you're looking at the right screen!

You can't buy the train tickets in advance (this is only possible for big important trains) but it is easy to buy them either from PisaMover in the airport or at the station, where you can ask a human ("Uno a Barga-Gallicano. Solo andata.") or one of the red, white, and green ticket machines, which can be requested to speak English. On all Italian train journeys you are supposed to validate ('convalidare') your ticket by inserting it into one of the small wall-mounted green and white machines in the station or you may have to pay a fine - though you should know that in ten years I have never seen a ticket inspector on any of the trains that you will take. Note that Italian trains are very (even absurdly) cheap by international standards, particularly British ones. The ticket should cost around 4 to 6 Euros.

One final thing that has caused confusion in the past: at Lucca and Pisa some of the trains leave from a platform labelled '1TO' or '1TE', meaning 1 Tronco Ovest (west) and 1 Tronco Est (east). This is *not the same* as Platform 1. All the 'through platforms' are labelled 1, 2, 3 etc., and 1TO and 1TE refer to separate 'terminus platforms' which you can find by walking to either the west or east end of Platform 1.

At Barga-Gallicano station you should find a TTI representative who will meet each Saturday train as required and take new arrivals to the Institute. If no-one is there you can wait in the station café - do call us if you find yourself waiting too long. Clearly we need to know in advance the time of the train on which you intend to arrive. The timetable is linked from the TTI web site, but all Saturday train times are in fact given in the table below. Note that the last train from Pisa is around 20:50 so it would be a good idea to arrive earlier in the day if possible (particularly if you want to enjoy the welcome buffet dinner at 19:30 - remember that staff members who have to pick up latecomers miss their dinner too!).

In emergencies - or if you arrive at an unusual time after the first day when our drivers might be busy - it is possible to get a taxi to Vallico Sotto from the station. In general this needs to be pre-booked - see the instructions on the web site (Barga Taxi : bargataxi@libero.it Tel. 331 3378051 or 339 5678336) but we can do this for you on request. If you are a non-Italian speaker who hasn't pre-booked and you need to talk to the guy (Massimo) on the phone you will find he doesn't speak English so just say (phonetic) "Taxi a Vallico Sotto da la statsionay di Barga-Gallicano?" or similar down a phone at him - the trip should cost around 35 Euro. Note that "I don't speak Italian" is "Non parlo italiano" - though I'm sure he can figure that out all by himself.

In case of problems contact Mike on his mobile - 00 44 7432 491113. (Additional emergency assistance may be available from Samantha Keil on 00 44 7979 554034 but she doesn't deal well with emergencies, so try to keep calm and

pretend everything's alright - screeching or hyperventilating or anything like that would probably be counterproductive, even if the train's on fire). TTI has two direct phone lines (0583 761608 and 0583 1805441) which you should use as a last resort, since the people you want are unlikely to be standing next to them.

3 TRAIN TIMETABLES

See http://www.trenitalia.com and click the British flag at the top right. Note that if you use the Italian version then it's important to click 'Tutti i Treni' (all trains) in the red box since by default the train look-up thing only gives you 'Le Frecce' (superexpensive intercity fast trains) - excellent example of bad web design.

Saturday 26th July, Pisa Centrale to Barga-Gallicano station

dep. Pisa	arr. Lucca	dep. Lucca	arr. Barga-Gallicano
05:25			06:47
06:13	06:39	06:55	07:37
07:50			09:19
10:20	10:47	11:26	12:08
12:50	13:17	13:26	14:17
13:43			14:56
15:20			16:37
16:20	16:44	17:00	17:46
17:50			19:06
18:50			20:32
19:50			21:40
20:50	21:17	21:48	22:27

Saturday 2nd August, Barga-Gallicano to Pisa Centrale station

dep. Barga-G.	arr. Lucca	dep. Lucca	arr. Pisa
05:55	06:40	06:52	07:16
06:40			08:13
07:23	08:11	08:50	09:16
08:49	09:34	09:42	10:13
11:55	12:46	13:12	13:43
14:09			15 : 43
15:23	16:10	16:42	17:13
18:51			20:14
20:26			22:13

3.1 From Milano

People coming from more distant countries often only have a choice of coming to Milano airport. Here is a summary of advice for them.

Travel from Milano Malpensa airport to Milano Centrale train station:

The Malpensa Express train departs from Terminal 1 for Milano Centrale train station around twice an hour. (One can also get to other Milano stations Cadorna, Bovisa and Saronno but Centrale is the main train station where you need to catch onward trains. Note that the Malpensa-Centrale line only opened in 2010 so you may still encounter outdated advice that you need to travel to Cadorna from the airport). The first train departs Malpensa at 05.43, the last train departs 22.56. Journey time is around 40-50 minutes. Fare: 10 Euro one-way. Best not to get in a taxi as it will cost you 65+ Euro.

Travel from Milano Linate airport to Milano Centrale train station:

This smaller airport is much closer to the centre than Malpensa, and therefore it is feasible to use buses or taxis to get to the train station. See the Linate Airport section of http://wikitravel.org/en/Milan for details about the various options.

From Milano Centrale train station to Barga-Gallicano

Saturday 26th July 2014

From Milano Centrale as above. Then choose one of the following trains - the 08:10 and 13:10 are probably best since there is only one change, and no later train will get you to Vallico Sotto in time for dinner. (There are other possibilities, but they involve tricky four-train connections, or getting up too early).

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OPTION 1 - (from 26.10 EUR) *** - BEST
Milano Centrale 08:10 --> Pisa Centrale
                                                         12:21
Pisa Centrale
                       13:43 --> Barga-Gallicano
                                                         14:56
OPTION 2 - (from 34.80 EUR) *** - SECOND BEST
Milano Centrale 13:10 --> Pisa Centrale
                                                         17:10
                       17:50 --> Barga-Gallicano
Pisa Centrale
                                                         19:06
OPTION 3 (from 16.10 EUR)
Milano Centrale 14:05 --> La Spezia Centrale
                                                         17:22
La Spezia Centrale 17:29 --> Aulla Lunigiana
Aulla Lunigiana 19:18 --> Barga-Gallicano
                                                         17:53
                                                         20:25
OPTION 4 (from 14.70 EUR)
Milano Centrale 16:05 --> Viareggio
                                                         20:00
Viareggio
                     20:10 --> Lucca
                                                         20:27
Lucca
                       20:53 --> Barga-Gallicano
                                                         21:40
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If you fly into Milano before Saturday, another option is to stay in a suitable hotel in Milano and take a train the day after. Before you arrive, write down the details of suitable hotels near the station. There is a good site where you can book these and print out maps at:

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http://www.traveleurope.it/milano.htm
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or better still:

http://www.traveleurope.it/milan/milan_central_station.shtml

The Hotel Monopole seems a good one to me (prices from 60 EUR)

4 SPECIFIC TRAVEL PLANS

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Lisa Johnson-Davies
Arr Pisa 14:45 Fri 25 July. Train dep Pisa 17:50 arr Barga-Gallicano 19:06
No departure - continue to summer school.
Elaheh Mostaani
Arr Roma 17:30 Fri 25 July. Train dep Roma Termini Sat 26 July 09:57,
                            arr Pisa Centrale 13:00. Dep Pisa 13:43
                            arr Barga-Gallicano 14:56
Dep Firenze 18:38 Fri 1 Aug (for flight Roma 4th Aug)
TO BOOK Roma-->Pisa 09:57 26 Jul (34.50 EUR)
       Firenze --> Roma 18:38 1 Aug (43.00 EUR)
Blazej Jaworowski
Train from Milano Sat 26 July, arr Barga-Gallicano 14:08 (pickup at 14:56)
Dep Pisa 14:08 Sat 2 Aug
Fionn Malone
Arr Pisa 11:35 Sat 26 July. Train dep Pisa 13:43 arr Barga-Gallicano 14:56
Dep Pisa ??:?? Sat 2 Aug
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Tom Poole

Arr Pisa 11:35 Sat 26 July. Train dep Pisa 13:43 arr Barga-Gallicano 14:56 Dep Pisa 19:20 Sat 2 Aug

Will Vigor

Arr Pisa 11:35 Sat 26 July. Train dep Pisa 13:43 arr Barga-Gallicano 14:56 Dep Pisa 22:15 Sat 2 Aug

Caterina de Franco

Train Sat 26 July arr Barga-Gallicano 14:56 No departure - continue to summer school.

Jonathan Lloyd-Williams

Arr Pisa 11:35 Sat 26 July. Train dep Pisa 13:43 arr Barga-Gallicano 14:56 Dep Pisa 22:15 Fri 1 Aug

Matthew Foulkes

Arr Pisa 12:05 Sat 26 July. Train dep Pisa 13:43 arr Barga-Gallicano 14:56 Dep Pisa 16:20 Thu 31 July

Shibing Chu

Arr Pisa Sat 26 July. Train dep Pisa 13:43 arr Barga-Gallicano 14:56 No departure - continue to summer school.

Tack Uyeda

Arr Pisa 19:40 24 July. Two nights Pisa. 26 July Train dep Pisa 13:43 arr Barga-Gallicano 14:56 Dep Sat 2 Aug (for Pisa Sun 3 Aug)

Cyrus Umrigar, Kyra Umrigar, Jasmine Umrigar Arr Livorno 13:15 Sat 26 July. Train dep Livorno 14:52 arr Pisa 15:09 Train dep Pisa 15:20 arr Barga-Gallicano 16:37

Dep for Rome Sat 2 Aug

Ching-Ming Wei

Arr Roma 09:36 Sat 26 July. Train Roma --> Pisa.

Train dep Pisa 15:20 arr Barga-Gallicano 16:37

Dep Fri 1 Aug pm.

Andrea Droghetti

Arr Sat 26 July Barga-Gallicano 17:33 (WAIT TILL 17:46 FOR PICKUP). Dep Fri 1 Aug (drop at Lucca)

Alex Haider

Arr Pisa Centrale 15:30 Sat 26 July. Train dep Pisa 16:20 arr Lucca 16:44 dep Lucca 17:00 arr Barga-Gallicano 17:46 [NO - NOW WANTS TO COME 10pm??]

Csaba Daday

Arr Pisa 15:30 Sat 26 July. Train dep Pisa 17:50 arr Barga-Gallicano 19:06 Dep Pisa 12:00 Sat 2 Aug

Mariapia Marchi, Sandro Sorella Arr by private car Sat 26 July, c. 16:30. Dep by private car Fri 1 Aug

James Shepherd

Arr Pisa 18:50 Sat 26 July. Take PLR rental car to TTI. Dep Pisa 20:05 Tue 29 July [MDT TO BOOK TAXI]

Pierre-Francois Loos

Arr Pisa 18:50 Sat 26 July. Take PLR rental car to TTI. Dep Pisa 15:10 Fri 1 Aug

Bartomeu Monserrat-Sanchez, Richard Needs, John Trail Arr Pisa 18:55 Sat 26 July. Take PLR rental car to TTI. Dep Pisa 22:15 Fri 1 Aug

Sam Azadi

Arr Pisa 18:55 Sat 26 July. Take PLR rental car to TTI.

Dep Pisa 17:45 Sun 10 Aug (staying to help with summer school).

Pablo Lopez Rios

Arr Pisa 18:55 Sat 26 July. Drive rental car to TTI (with SA/BMS/RN/JS/JRT,PFL) Dep Pisa 19:20 Sat 2 Aug

Edgar Engel, Gareth Conduit

Arr Pisa Sat 26 July. Train to Barga-Gallicano. Pick up MDT's Peugeot 106 from the secondary car park (follow the path from the south end of the platform).

Dep Pisa 22:15 Fri 1 Aug

Ryo Maezono, Kenta Hongo Arr Sat 26th July pm by private car Dep Fri 1 Aug by private car

Giovanni Bachelet Arr Sat 26th July pm by private car Dep Fri 1 Aug by private car

Dario Bressanini Arr Sat 26 July by private car Dep Fri 1 Aug pm by private car

Dario Alfe

Arr Sat 26th July pm by private car Dep Mon 28th July pm by private car

James Spencer

Arr Sun 27th July by train arr Barga-Gallicano 19:06. MDT TO BOOK TAXI TO SANDRA Dep Pisa Sat 2nd Aug

Leonardo Guidoni Arr Sun 27 July by private car Dep Wed 30 July evening

Alex Thom

Arr Pisa 11:35 Mon 28 July. Train dep Pisa 12:50 arr Lucca 13:17 dep Lucca 13:26 arr Barga-Gallicano 14:17 TAXI BOOKED

Dep Sat 2 Aug

Martin Korth Arr Mon 28 July pm by private car Dep Fri 1 Aug pm by private car Ron Cohen

Arr Mon 28 July pm by private car

Dep Fri 1 Aug by private car

Nic Harrison

Arr Pisa 21:55 Monday 28 July by private car.

Dep Pisa 21:15 Wednesday 30 July by private car.

Neil Drummond

Arr Pisa 12:00 Tue 29 July. Train dep Pisa 13:43 arr Barga-Gallicano 14:56

No departure - continue to summer school.

Carlo Pierleoni

Arr Wed 30 July by private car

Dep Sat 2 Aug

Roberto Dovesi

To be confirmed. University duties..

5 ACCOMMODATION

TTI, ATTIC - one single mattress, one cot $\operatorname{\mathsf{Mike}}$ Towler

TTI, NURSERY - one single bed Jamie Towler

TTI, PLAYROOM - two single beds, one double bed Neil Drummond, Pablo Lopez Rios

TTI, PINK ROOM

Samantha Keil, Saska Towler

TTI, LILAC ROOM - two single beds Caterina De Franco, Mariapia Marchi

TTI, TINY ROOM – one single bed ${\tt James}$ Spencer

TTI, RED ROOM - one double bed Richard Needs

TTI GARDEN ROOM - two single beds (bunk) Lisa Johnson-Davies, Alex Haider

DOCTOR'S HOUSE, FIG TREE ROOM - one double bed Matthew Foulkes

DOCTOR'S HOUSE, UPPER TWIN ROOM - two single beds Kenta Hongo, Ryo Maezono

DOCTOR'S HOUSE, FIRST UPPER ROOM - one double bed

Alex Thom

DOCTOR'S HOUSE, LOWER APARTMENT - one double bed, two single bunk beds Cyrus Umrigar, Kyra Umrigar, Jasmine Umrigar

CASA FRANCA - ROOM 1 - 1 double bed Shibing Chu

CASA FRANCA - ROOM 2 - 1 double bed John Trail

CASA FRANCA - ROOM 3 - 1 double bed Sandro Sorella

CASA FRANCA - ROOM 4 (ATTIC) - 1 single bed Edgar Engel

CASA GIANPIERO - ROOM 1 - one double bed Giovanni Bachelet

CASA GIANPIERO - ROOM 2 - two single beds Dario Bressanini Martin Korth

CASA LUCIANA - ROOM 1 - 1 double bed Tack Uyeda

CASA LUCIANA - ROOM 2 - 1 single bed Bartomeu Monserrat-Sanchez

CASA LUCIANA - ROOM 3 - 1 sofa bed Jonathan Lloyd-Williams

CASA SARDA - 1 single bed Ron Cohen

CASA GIOVANNI - ROOM 1 - 1 double bed Ching-Ming Wei

CASA GIOVANNI - ROOM 2 - 1 double bed Pierre-Francois Loos

CASA GIOVANNI - ROOM 3 - 2 single beds Gareth Conduit

CASA LIANA - ROOM 1 - 1 double bed Sam Azadi

CASA LIANA - ROOM 2 - 2 single beds Csaba Daday, Andrea Droghetti

CASA LONTANA - ROOM 1 - 1 double bed, 1 single bed Will Vigor, Fionn Malone

CASA LONTANA - ROOM 2 - 1 double bed Blazej Jaworowski

CASA LONTANA - ROOM 3 - 1 single bed

Tom Poole

BEDOUIN TENT (www.vallico.net/tti/tti_tent.html)

DA SANDRA (multiple commercial rooms: dasandra.jimdo.com)

Local restaurant offering private rooms and apartments at a reasonable price - 3 minute drive / 15 minute walk - more suitable for people with cars but transport will be arranged even for people without. Please pay the owner directly (Sandra's daughter Serena is responsible for accommodation at the restaurant) but ask MDT to book the room. Cost : 60 Euros per night.

DA SANDRA - ROOM 1 - 1 double bed James Shepherd (Sat, Sun, Mon night only..) Nic Harrison (Tue)

DA SANDRA - ROOM 2 - 1 double bed Elaheh Mostaani (Sat, Sun, Mon, Tue, Wed, Thu)

DA SANDRA - ROOM 3 - 1 double bed Dario Alfe (Sat, Sun night) Carlo Pierleoni (Wed, Thu, Fri night)

DA SANDRA - ROOM 4 - 1 double bed Leonardo Guidoni (Sun, Mon, Tue)

CASALE DEI RUSCELLI (www.casaledeiruscelli.com)

Lovely apartments for rich people requiring privacy - 12 min drive - car and extra payment required. Please pay the owner directly - but ask MDT to book this.

HOTEL CRISTALLO - CHEAP NASTY HOTEL IN FORNACI DI BARGA (25 min drive)

VILLA MOORINGS - EXPENSIVE POSH HOTEL IN BARGA (30 min drive) http://www.villamoorings.it/

AWAITING ASSIGNMENT OF ACCOMODATION Roberto Dovesi

6 CONFERENCE VEHICLES

Max 47 people to transport simultaneously; 37 official seats plus 50 private (30 temporary)

OFFICIAL VEHICLES

17-seater bus - driver: Mike Towler 9-seater rental car - driver: Pablo Lopez Rios

6-seater Fiat Multipla - driver: Sam Azadi 5 seater Peugeot 106 - driver: Edgar Engel

PRIVATE VEHICLES

5 seater rental car - Martin Korth 5 seater rental car - Ron Cohen 5 seater - Mariapia Marchi

OTHER PRIVATE VEHICLES PRESENT FOR PART OF THE WEEK:

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5 seater private car - Giovanni Bachelet (leaving 1 day early)
5 seater private car - Ryo Maezono (leaving 1 day early)
5 seater private car - Dario Alfe
5 seater private car - Ron Cohen
5 seater private car - Leonardo Guidoni
5 seater private car - Nic Harrison

SPARE DRIVERS (please bring driving license):
None needed.
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7 THINGS TO BRING WITH YOU

- The slides for your talk if you intend to give one see later section for supported formats.
- Your laptop, if you wish (though this is completely not necessary, as we have large numbers of them see note in Technical Equipment section). That said our official laptops mostly bought years ago when MDT still had a budget are now starting to die. We have lost five of them to electronic failures in the last couple of years and we can longer replace them. So if you have old laptops you would like to donate to the Institute these would be very welcome (and would be particularly useful for the associated QMC summer schools).
- Summer hiking gear such as boots, socks, little rucsacs, sunhats etc.
- Italian plug converters if you want to plug anything in (we have some spare but donations of these are gratefully accepted). Our sockets mostly have two round pins (with an optional third one between them). There are two types of thin prongs on European adaptors. You want the thinner of the two. Just to confuse things, there are also lots of totally incompatible English plug sockets into which English equipment can be plugged directly.
- Some Euros for spending in restaurants and shops (mininum 25 Euros per day). Please note that there is no cash machine within walking distance of the Institute, and although we might pass them from time to time on our afternoon trips, large numbers of people getting money out can cause considerable delays. There is a cash machine in Pisa airport to your left as you emerge into the arrivals hall (look under the escalator leading to the upper level). Go up the escalator to find an alternative cash machine if that one isn't working. A few years ago a cash machine was in fact setup in Fabbriche di Vallico a few kilometres away from the Institute, and it now usually works this is where you should go if you run out of cash during the week (if you can't find it, find a local and say 'Bancomat?').
- People who intend to visit caves or canyons should bring some clothes and old shoes that you don't mind getting
 wet.
- Climbing/caving equipment (harness, boots, helmet, via ferrata 'absorber', head torch) if you intend to take part in such activities and already have some (don't buy them just for this trip). We have a fair amount of gear we can lend but not enough for everyone.
- Light sleeping bag and a torch (if you intend to sleep in the Bedouin tent).
- Hay fever tablets. Some people who have lived in darkened basements in huge cities most of their lives sometimes have difficulty with pollen when they come to live in the countryside.
- A musical instrument, if you can play a portable one. See Section 15.
- Sunscreen. It is likely to be quite hot in the first week of August, but note that because we are in the mountains occasional afternoon rain showers are not unknown.
- A towel
- Swimming costume (if you wish to go swimming).
- Earplugs if you are sharing a room to avoid being disturbed by snoring people.

In the tradition of earlier workshops, you might also optionally like to bring

- A nice bottle of wine (or whatever passes for it in your country).
- An interesting thing

Friday 25th July

8 CONFERENCE SCHEDULE

This section contains the schedule for the conference, including a list of talks. The number of talks per day is deliberately small to allow time for thinking, discussion and deliberation. In principle there could be evening discussion sessions if required. If you do not wish to give a talk, or if you wish to give a shorter/longer talk than suggested, please ask. All excursions and activities are, of course, optional - and you may elect simply to relax at the Institute in the afternoons though then transport to the evening restaurant will need to be arranged. We have to book restaurants well in advance for such large groups so please make it known in good time if you do not wish to attend particular meals.

Note that on arrivals day Sat 26th July a daring, strenuous, and possibly even dangerous mountain excursion for volunteers will be arranged if there is sufficient interest - let MDT know if you want to go along. In the past this has included things like the ascent of Pizzo D'Uccello (the Matterhorn of the Apuan Alps) - a similar suitable excursion will be made up nearer the time when it's clear who's going.

Note that the list of 'Possible Excursions' is intended only as a guide to typical things that might go on. What actually happens on the afternoon of any given day is usually made up by MDT during the morning; he is always very open to suggestions and requests. There is an 'independent excursion cupboard' with maps and guide books to help you.

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EARLY ARRIVALS
Erection of Bedouin Tent.
Systems testing.
DINNER: TTI kitchen for anyone arriving early
Saturday 26th July
ARRIVALS
Strenuous excursion e.g. Pizzo d'Uccello for people who arrived yesterday.
Current volunteers: Mariapia Marchi, Sandro Sorella
INSUFFICIENT INTEREST - CANCELLED.
7.30pm : TTI 10th Anniversary Welcome party and buffet on the Doctor's Lawn.
Featuring Ed the Singer, an Elvis 1950s microphone, TTI's new PA system, and a
large selection of light jazz standards sung on request. Entire population of
Vallico Sotto to be invited.
Sunday 27th July
8.30am : Pablo Lopez Rios (50 minutes)
       - "Multideterminant compression"
9.30am : Dario Alfe (25 minutes)
       - "Water clusters, ice, and bulk liquid: improving ab initio structure
          and energetics"
10.00am : Cyrus Umrigar (50 minutes)
       - "Semistochastic quantum Monte Carlo -- A hybrid of exact
          diagonalization and quantum Monte Carlo methods"
11.00am : Bartomeu Monserrat-Sanchez (50 minutes)
       - "An overview of vibrations in solids"
12.00am : Csaba Daday (25 minutes)
        - "Wave function embedding methods and excited states: A guide to the
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perplexed"

12.30pm : CHURCH (if you want)

- A DAY IN THE VILLAGE TO REST AFTER YOUR LONG JOURNEYS
- Relaxing, sunbathing, reading, studying, discussing

POSSIBLE EXCURSIONS:

- Nice figure-of-eight tour of Vallico Sotto, Vallico Sopra, and San Luigi (convertible to the a circular tour of the Vallicos for the physically challenged).
- Turrite di San Rocco canyon walk
- Mule trail clearing
- Independent cave-hunting (ask Mike)

DINNER: Da Sandra (BOOKED FOR 41)

Monday 28th July

- 8.30am : Sandro Sorella (50 minutes)
 - "Ab initio simulation of liquid water by quantum Monte Carlo"
- 9.30am : Pierre-Francois Loos (50 minutes)
 - "Chemistry in a 1D world"
- 10.30am : Ryo Maezono (25 minutes)
 - "DMC calculations for electron and electron-hole gases"
- 11.00am : Will Vigor (25 minutes)
 - "Unloading the dice: minimising biases in full configuration interaction quantum Monte Carlo"
- 11.30am : James Shepherd (25 minutes)
 - "Data driven analysis of the sign problem in full configuration interaction quantum Monte Carlo"
- 12.00am : Fionn Malone (25 minutes)
 - "Parallel strategies for FCIQMC"

POSSIBLE EXCURSIONS:

- Walk Matanna to Monte Forato (rock arch) to Fornovolasco new ferrata route
 Tana che urla cave
- Walk Palagnana-Monte Croce-Fornovalasco
- San Pellegrinetto Walk led by Mountain Guide Saska Towler
- Grotta del Vento tourist cave
- Fornovolasco church and flood frescoes
- Independent cave-hunting (ask Mike)
- Swimming at Barga

DINNER: New Eremo di Calomini (BOOKED FOR 42)

Tuesday 29th July

- 8.30am : Alex Thom (25 minutes)
 - "FCIQMC and finite electron gases"
- 9:00am : James Spencer (25 minutes)
 - "An overview of the HANDE QMC project"
- 9.30am : Leonardo Guidoni (50 minutes)
 - "Geometries and properties of (bio) molecules by Quantum Monte Carlo"
- 10.30am : Gareth Conduit (50 minutes)
 - "Pseudizing the Hamiltonian"
- 11.30am : Ching-Ming Wei (25 minutes)
 - "Binding energy of 2D materials using QMC"
- 12.00am : Jonathan Lloyd-Williams (25 minutes)
 - "DFT and QMC calculations of solid molecular hydrogen"

POSSIBLE EXCURSIONS:

Trip to Alto Matanna. Numerous spectacular walks of varying difficulty. See the Versilia coast, Elba, Corsica and sometimes even France from the easily accessible summits of some of the more beautiful scenery in the Apuan Alps. Bring one of the Institute's antique telescopes to watch the more courageous of you scale the 500 foot cylindrical barrel of Monte Procinto. Followed by drinks and dinner in 19th Century Alpine hotel.

- Balloon station walk (short and easy)
- Monte Matanna walk (medium) possible extended to Monte Nona.
- Monte Procinto climb (strenuous)
- Monte Croce circular walk from Palagnana (strenuous)
- Grotta all'Onda walk (Neanderthal cave) (very strenuous)

DINNER: Matanna (BOOKED FOR 43)

Wednesday 30th July

- 8.30am : John Trail (50 minutes)
 - "Pseudopotentials for correlated electron systems"
- 9.30am : Nic Harrison (50 minutes)
 - "Describing strong interactions some outstanding problems"
- 10.30am : Tom Poole (25 minutes)
 - "Algorithmic differentiation of diffusion Monte Carlo"
- 11.00am : Ron Cohen (50 minutes)
 - "Quantum Monte Carlo simulations on silicate perovskite and other high pressure phases"
- 12.00am : Edgar Engel (25 minutes)
 - "Anharmonic nuclear motion and the relative stability of hexagonal and cubic ice"

POSSIBLE EXCURSIONS:

- Monte Sumbra
- Coreglia di Antelminelli and Buca delle Fate
- Swimming and shopping in Bagni di Lucca

DINNER: Al Laghetto (BOOKED FOR 42)

Thursday 31st July

- 8.30am : Richard Needs (50 minutes)
 - "Xenon oxides under pressure"
- 9.30am : Elaheh Mostaani (25 minutes)
 - "Binding energy of bilayer graphene (updated) and electronic properties of oligoynes"
- 10.00am : Martin Korth (50 minutes)
 - "On the hunt for molecular organic battery materials"
- 11.00am : Kenta Hongo (25 minutes)
 - "QMC applications to noncovalent interactions in cyclohexasilane dimers"
- 11.30am : Andrea Droghetti (25 minutes)
 - "Spin-crossover molecules: puzzling systems for electronic structure methods"

A DAY IN THE VILLAGE

- Relaxing, sunbathing, reading, studying, discussing
- Metal detecting
- Orienteering
- Abseiling to the Buca della Fate di Vallico di Sotto
- Football match Vallico Sotto against the world/Vallico Sotto contro il mondo

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DINNER: Provided by Federico and friends at Vallico Sotto (BOOKED FOR 39)
MUSICAL EVENING back at the monastery afterwards
Friday 1st August
8.30am : Carlo Pierleoni (50 minutes)
        - "Liquid-liquid phase transition in high pressure hydrogen: new
          predictions from CEIMC and comparison with DFT"
9.30am : Neil Drummond (50 minutes)
        - "Electronic and vibrational properties of monolayer hexagonal
          indium chalcogenides"
10.30am : Tack Uyeda (25 minutes)
       - "Estimation of exchange interaction of SrMnO3 by QMC"
11.00am : Mariapia Marchi (25 minutes)
        - "Using modeFRONTIER to automate DFT and QMC calculations:
           application to liquid hydrogen"
11.30am : Mike Towler (50 minutes)
       - "High-throughput QMC"
POSSIBLE EXCURSIONS:
- Lucca
- Orrido di Botri
DINNER: Make your own pizza evening at TTI (FOR 25 PEOPLE)
        If you go on the Lucca trip, please visit the delicious
        independent food shops and buy nice things for the evening dinner.
        Mike will be buying his favourite Barolo-soaked cheese.
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Saturday 2nd August

DEPARTURES

NO TALK: Matthew Foulkes, Sam Azadi, Blazej Jaworowski, Giovanni Bachelet, Dario Bressanini, Shibing Chu, Caterina de Franco, Roberto Dovesi

TTI TECHNICAL EQUIPMENT

There are various modern laptop computers in the Institute available for general use. Most offer some recent version of OpenSuse or Ubuntu Linux, with only a few left (those kept out of the hands of our anti-Microsft activist Pablo) still able to dual boot into Windows XP/Vista/7. You may of course bring your own laptop if you wish. Please be careful of the dodgy electrics when plugging in your own machine in order to avoid shorting out the projector etc. - in fact, it's better to ask where to do so. Note that most of the available plug sockets in the lecture hall are of the English type though some Italian ones are available.

All internet connections are made - via a dish on the roof - through a high quality wireless network (the TTI infrastructure was comprehensively upgraded in June 2014). In fact, because of the wide area covered by the monastery and because of its ancient 5 feet thick stone walls, there are actually 4 wireless networks on different frequencies (which cooperate and do some clever balancing tricks via a very clever box with flashing lights in the attic). The SSIDs are "TTI_Church', "TTI_1', "TTI_2', and "TTI_3' with a common WEP password 'vallicochurch'. If any particular laptop appears not to be connected to the network, then right click on the wireless icon in the bottom left-hand corner (OpenSuse Linux) or top-right (Ubuntu) and click on the 'TTI_Church' connection.

Apart from computers and networking devices, we also have the following equipment available:

- A HP Laserjet black and white printer (on a wireless print server at 10.0.4.10, so one can print from anywhere in the Institute). The relevant print queue is called 'hp'.
- Canon Pixma ip4000 colour inkjet printer
- Hi-Ti Transphotable and Sony photo printers for instant printing of your photographs (you can plug in your camera directly - no need to go through a laptop - accepts all memory card formats that I am aware of). Note that we have limited supplied of the expensive paper and ribbons, so try not to print off your entire collection.
- Epson Perfection 4990 scanner (usually upstairs in main building near MDT's desk).
- A3 laminator
- Guillotine
- A HD video camera
- Four or five USB memory sticks (labelled TTI)
- A supply of writeable CD-Rs, CD-RWs and DVD-Rs.
- The usual stationery, staples, paper..

There are also a very large number of scientific and technical books which may be borrowed (top floor of the main building, and in the various bookshelves in the church).

Please note that there is also a pigeon-hole bookcase intended for printouts of 'the literature'. At the moment this still contains all the relevant papers for '21st-century directions in de Broglie-Bohm theory and beyond' - a huge conference we ran a couple of years ago, but it may be refilled with anything you like. You are welcome to borrow these papers, but please put them back in the same place you got them from as they are all carefully filed..

10 INTERNET USE

TTI laptops are mainly black/grey Sony Vaios with a few red Acer Ferraris (note the difference in power supplies - the ones for the Ferraris have yellow ends, the Sony machines have black ones). All should connect themselves to the wireless network as soon as they've finished booting up.

The monastery's local network connects to the outside world through the wireless broadband network using the CloudItalia service. Young people should note how lucky they are; TTI was necessarily on dialup (!) for the first few conferences before 2009 - meaning that the front page of a typical modern newspaper would take about 5 minutes to render...

All local machines have static IP addresses 10.0.4.2x on the TTI_Church network (where 2x is 20 plus the number of the machine - a red plastic label saying e.g. tti_laptop9 implies 10.0.4.29) so they can all talk to each other via ssh or ftp etc. With appropriate software all the laptops can be run as a parallel supercomputer in the unlikely event of someone needing to do some QMC calculations with the link to the outside world cut off.

Other network details for administrators: TTI_Church network: IP 10.0.4.xx (static xx=10-99, DHCP assigned numbers from xx=102-254), Gateway 10.0.4.1, Primary DNS 8.8.8.8, Secondary DNS 62.94.0.1.. The router has a (password protected) web page at 10.0.4.1, the access point at 10.0.4.2. For the TTI_1, TTI_2, TTI_3, and TTI_5 networks, replace the 4 in the TTI_Church IP with 1,2,3,5... Other equipment attached to the network: a phone adapter, a wireless range extender (possibly), internet radio attached to TTI_1, a wireless print server (10.0.4.10, print queue 'hp'), and possibly the NEC projector on DHCP. Do not assign your own static IP number on personal hardware without consulting MDT.

There is a central file server (a Synology DS1513+ 5 Bay DiskStation Desktop NAS with 10 TB of storage) attached directly to the main router box on 192.168.1.200. Access to this can be provided on request for local events.

Please be mindful of the needs of other users of the network. Although we have an excellent connection, it is clear that most people are now turning up with WiFi-enabled smartphones and tablets, and it remains to be seen whether things will scale up to allow 60 people to do this, whilst using 30+ laptops and all the other stuff.. The network was upgraded this year for precisely this reason, but it is gently suggested that downloading Gb of files, playing streaming music or videos through your smartphones, enabling automatic software updates, might not be a good idea.. Remember we're in the middle of nowhere - it's amazing that it works at all!

Note also that currently there is network coverage only in the main TTI building and garden, and in the Luxury Bedouin Tent, but not in any of the other houses we use for accommodation (Doctor's House, Casa Franca, Casa Gianpiero, Casa Luciana, Casa Sarda, Casa Lontana). An extension to the Doctor's House has been ordered, and this will hopefully be physically enacted before the conference (the network people are a bit behind schedule because of recent bad weather..).

The local network is normally configured to believe it is part of Cambridge University via their VPN service. This is very useful for e.g. accessing restricted content scientific articles. Sadly, Cambridge rules prevent us provided such access to TTI visitors, and so the VPN is normally turned off during conferences. Ask MDT if you want to make (indirect) use of this service.

11 PRESENTATION EQUIPMENT

The church is equipped with a good quality NEC MT1075 projector and an auxiliary Toshiba DPD TDP-T250U projector with DVI and regular RGB cabling. There is a giant 16' by 12' main screen, a 7'8 x 5'9 electric auxiliary screen, an Avervision document camera, a dual projection stand, a laptop, a DVD player with decent speakers, and various wireless control devices. There is a giant blackboard in the church and a smaller one in the lower main corridor of the main building stolen from the TCM Seminar room in the Cavendish Laboratory. There are two blackboards outside, and a portable one which can be taken on excursions if you wish to debate physics in restaurants or up mountains.

The NEC projector is wireless capable, so you can beam your talk from your laptop straight to it from anywhere in the room, as well as with old-fashioned direct connection (technical specs on the TTI website). The Institute projection laptop - though normally bootable into either Linux or Windows - will normally be running under Windows because Linux Powerpoint viewers mostly do not display Microsoft-generated files correctly. Obviously it will accept CDs and memory sticks and have the usual software such as Acroread and Powerpoint. On balance it is probably best to bring your talk on a CD or USB device or email it to MDT beforehand and he will ensure that it is on the projection laptop ready for your talk. We would be grateful if you could leave your talk on the Desktop of this machine so that your talk can be made available (password protected if you request it) on the conference web page after you've all gone home.

The Avervision document camera is a sort of cool overhead projector. It will display any printed document, photo, slides, X-ray film or 3D object straight through the projector, so basically you can dissect a frog live on the wall. There is a Victorian microscope with an attachment that allows it to be connected to the Avervision, so biological people can project the microworld on the big screen. Although we have a table with a white square painted on it, non-electronic talks are probably better on white pieces of paper rather than on transparencies..

12 EXCURSIONS AND ACTIVITIES

The various excursions and activities are divided into categories according to the physical effort involved. As there will be around 40 people at the conference, it is envisaged that each day the group will split into two or more subgroups, with the hot young muscular virile people doing the strenuous excursions, and the lazy, old and unfit doing more relaxed activities. Although we have incorporated suggested activities into the programme above, everyone is welcome to consider the following list and also to consult the various guidebooks in the TTI library in order to suggest alternative activities.

12.1 Very strenuous activities

- Climb the peak of Pizzo d'Uccello. Requires early start with no other activities (e.g. day before conference). See http://www.tcm.phy.cam.ac.uk/~mdt26/tti2/photos/pizzo_duccello.jpg. Enough said. They don't call it the 'Matterhorn of the Apuan Alps' for nothing.
- The ascent of Monte Procinto. This is a huge cylindrical rock tower with a belt of trees around its middle from which rise 500-foot walls, overhanging on every side. Michelangelo had the idea of carving it into a gigantic scultpure along the lines of Mount Rushmore but never got round to it. You can see the mountain here: http://vallico.net/procinto.jpg or http://vallico.net/casinoqmc/wp-content/uploads/2014/01/procinto.jpg. Yes the walls are more or less vertical, but there is a *via ferrata* to clip yourself onto. Instruction, assistance, and the necessary equipment can usually be supplied but we only have about eleven harnesses so bring your own if you have one!

- Reach the high peak of Pania della Croce from Piglionico (described as 'The finest peak in the whole of Italy' in *Below the Snow Line* one of the 19th century books in the TTI Antiquarian Library). Also features in Dante's *Divine Comedy*. This defeated some of TTI finest mountaineers for several years before they finally succeeded in 2007 (note it isn't that hard if you move quickly).
- Find the spectacular natural rock bridge of Monte Forato (under which someone once flew a biplane). Start from Fornovolasco (lots of up) or from Matanna (much easier) or even have two groups that meet in the middle and exchange car keys. There is a fun via ferrata traverse on the way to the arch from Matanna, and we can also do a new route via Foce di Valli.
- Find the Neanderthal cave (Grotte all'Onda) down the slope from the balloon station near Matanna. "This vast grotto stretches 40 x 60 meters and it originally hosted numerous internal tunnels, which are obstructed today. Its enormous cavity offers important evidence that suggests the frequency with which people entered the grotto, from pre-historical times to more recent periods. The first people to use the cave were Neanderthals; they hunted throughout the surrounding area and probably used it to hoard their tools and weapons, together with the bones of the animals they cooked. Hunters from the Superior Palaeolithic period (Homo Sapiens) lived in the more external part of the grotto where they set up a giant hearth. Later, Neolithic farmers and shepherds planted their huts in the shelter of the grottos vast vault, carrying out their daily activities there during many seasons. This cave was also used during the Neolithic period (the Bronze Age), during which new models were developed for decorating ceramic. During this period, new raw materials, imported from distant locations, were adopted to make special equipment. From the post-Bronze Age until recent times, the grotto was not continuously frequented."
- The *Geoscopio* web site linked from http://vallico.net/tti/tti_mountaineering.html shows precise locations of all of the thousands of caves in Tuscany (even the crap ones) together with a brief technical description and a plan of the cave. Interesting little expeditions may be made that have the aim of finding the entrance to particular caves, as well as exploring them. This is of course the most fun that a boy can have. The Apuan Alps have more caves than you can possibly imagine, so this will still be a viable activity in 2050. In particular, ask Mike about the untried Campolemisi, Fabbriche di Vallico, Motrone, and Antro della Paura expeditions.
- Explore the canyon of the Turrite di San Rocco river. This starts from the fork in the river upstream from Fabbriche di Vallico before you get to Gragliana. Take the left-hand fork. The aim is to go all the way through it to take coffee at the cafe near the Chiesa di San Rocco in Turrite. Be prepared to get wet you basically can't avoid it. There are various natural swimming pool in there. Once reaching the village where the cafe is (there is also a children's playground and a nice river) you will have to bribe a local to give your driver a lift back via Focchia to your van. Or perhaps all your drivers drove a convoy out there beforehand, left most of the vehicles, and returned to the start of the canyon in a single car use your initiative here.
- Morning workout. Run from the Institute each morning at 6am to the spectacular summit of Monte Palodina in order to tone up your thigh muscles and pep yourself up in preparation for the morning's talks. Mad people only.
- Complete the Cinque Terre coastal walk, a four-hour excursion through some of Italy's most spectacular scenery, or a similar walk near the famous seaside haven of Portofino.
- Orrido di Botri canyon walk. The Orrido is a giant canyon created by the Pelago river in the Appenines (about an
 hour's drive from the Institute) with deep steep walls as high as 200 metres and in some places only a few metres
 apart. This is a geologists' and naturalists' paradise. It can only be visited with helmets and suitable clothing you
 don't mind getting wet. There are some nice long walks in the country above the canyon (watch out for marmites
 and Royal Eagles this is one of your best chances to contribute to the TTI Wildlife Photography expedition).
- There are of course any number of spectacular high mountain expeditions in the Apuan Alps and the Institute has a library of guidebooks which you can browse through. Let me know if you want to try anything else (that will fit in the clearly limited amount of time). There is also the TTI Antiquarian library (Mountaineering section) to inspire you.

12.2 Quite strenuous activities

• Go to Alto Matanna at the end of the Turritecava valley and visit the beautiful nineteenth-century hunting lodge that was once the destination for travellers in Rosetta the Balloon on her aerostatic cableway. See the old balloon station at Foce del Pallone and the extraordinary view. On clear days you can see Elba - 100 miles to the South - and sometimes the even more distant Corsica and the French Alps. Come back over the top of Monte Matanna and descend back to the lodge. Take one of the Institute's antique telescopes with you.

- From the Matanna hotel, climb up to the cross on the adjacent ridge for a spectacular view of Monte Procinto, Stazzema and the Apuan Alps. From there you can climb Monte Matanna the other way around, or visit the donkey and his little horse friends who live on the top of Monte Nona. Or you could go on a longer walk below the Giant West Wall of Nona, threading past Monte Procinto, and round the back of Monte Nona which will take several hours. Finish up the day with a fabulous dinner in the Matanna hotel.
- Take part in the latest expedition to the ancient cave known as the *Tana di Cascaltendine* which is the subject of Pietro Magri's 1880 book *An expedition to Mount Gragno and the Cave of Cascaltendine* as translated by Mike and available on the TTI web site (click the Local History Projects link). The 2007 summer school crew were able to photograph the result of the following quote: *'Before coming down from the cavern we used a chisel to inscribe our initials and the year 1880 on both walls of the passage near the entrance.*'. This was done in the "Palace of Ismeno" which was the name Magri's group gave to an extensive cave whose entrance is a 6 foot hole about forty feet up a cliff the full story is on the News from the Towler Institute blog here: http://www.barganews.com/blogs/towler/?p=21. It is also known that the cave continues for a kilometre beyond where we have penetrated before and this remains to be explored (note that in summer 2007, Mike and Evans went up the big wall in the final chamber with the dangling rope a place many TTI visitors have visited before with somewhat amusing conesquences see the blog story 'Bronze Hermaphrodites and the Fat Boy Filter': http://www.barganews.com/blogs/towler/?p=28). Expedition to be followed by cold beers and refreshments in the lovely village of Cardoso, or a circuit of Monte Penna hunting for the lost Cave of the Fairies..
- Visit the Selva del Buffardello adventure park:

http://www.selvadelbuffardello.it/index.php?lang=eng

I quote from their web site: "Among the centuries-old fir trees some acrobatic forest paths, open to everybody, have been created and their aim is to show the wood from a different and adventurous point of view: hanging in the air. It is a challenge for children, youth and adults, who can test their ability with suspension bridges, swinging beams, vertical nets, ropes and obstacles, finding again their lost adventurous spirit. The Adventure Park 'Selva del Buffardello' in San Romano in Garfagnana (locality Pra' di Lago) is a real novelty in the Appennino Tosco Emiliano. An old wood of two hectares and a half in the heart of Garfagnana, near the natural 'Parco dell'Orecchiella', with a wonderful view on the Alpi Apuane and on the Fortezza delle Verrucole (old castle). The park entrance is free if you don't practise in the adventure paths." We have never tried this, but it looks like great fun, even for grown-ups.

- TTI management has discovered that there is a secret underground tunnel in Vallico which starts from the Doctor's House next door to the Institute (a former barracks) and which goes up to the Rocchetta above the village (the site of an old castle on the summit of a little hill, where we now pitch the Bedouin Tent). This was used in mediaeval times for escape from the frequent warfare so common in these parts. The supposed entrance to the tunnel was bricked up (we think) in the 1930s there are a couple of elderly men in the village who vaguely remember it. This summer we hope to unblock the entrance and explore. We also wish to find the upper entrance, so if you know anyone who has a ground-penetrating radar set we can borrow, let us know. This will probably be one of the next thrilling tales in 'News from the Towler Institute'.
- Explore the Vallico Sotto mule trail and the spectacular forgotten waterfall of Cascata Pendolina one of the highest in Italy. Vallico was only connected by road to the outside world in the 1960s before then people went up and down the *mule trail*. This has now been forgotten and is a little overgrown (though less so following TTI clearing activities) but is still very beautiful. Once we reach the bottom of the valley we will head over the river to the site of the Cascata Pendolina where will take lunch. On the way back the bravest people will try to ascend the *Canyon of the Pili* carved by the Rio Selvano (you will get wet!). EDIT: and they will fail I have recently discovered the only way you can feasibly do this is to *descend* from the top. Apparently this canyon is quite famous the Apians group from Castelnuovo organize tours through it. One of these days I will have to attach myself to one of these expeditions to learn how to do it. Apparently there are 12 major waterfalls to descend photos and rough maps are linked from the Mountaineering page of the web site.
- Explore *Buca della Freddana* cave near the mule trail from Vallico Sopra to San Luigi. This was (re-)discovered by Mike in Easter 2007 following conflicting and confusing advice from several local old ladies who remembered its existence from 40 years ago. He has also found the upper entrance of the same cave on the summit of Monte Penna the two are apparently connected by a 1 kilometre passage. The old ladies have advised us not to go inside because of the evil monsters and dark pits that lurk within, but then again, they always say that. Dare you explore?

- Five a side-football (a new fenced pitch was constructed in Vallico a couple of years ago) or regular football (on the local full-sized pitch).
- Rock climbing or low-level bouldering the Institute should have some ropes and climbing equipment. I've read
 that there is good climbing near the Trombacco damn in the next door Fornovolasco valley ask MDT for more
 details. Don't forget to bring climbing boots and a harness that fits if you want to do this seriously (we have a
 rope you can borrow).
- Pietro Magri in his 1880 book mentioned above states that there are two other caves in Monte Gragno besides the Tana di Cascaltendine. Today no-one seems to know where they are. Having found the Buca della Freddana, Mike has narrowed down the lost "Cave of the Fairies" to a relatively small area. Can you find it?
- Traverse from Santa Luigi via Monte Palodina and the cliffs of Monte Gragno past the giant karst depression of Pian di Lago to the spectacular Rocca Estense fortress of Trassilico. Come back along the road past La Fornace.
- Explore the *Tana che urla* (the Cave that Screams!) first explored and scientifically described by Vallisneri in 1726 off the footpath to Foce di Petrosciano from Fornovalasco. This isn't a tourist cave suitable for your mum so bring some appropriate clothes and torches. By the summer the Institute should have some proper speleological equipment to hand round. If you can read Italian, have a look at http://lnx.buffardello.it/images/file/DI_ALCUNE_GROTTE.pdf
- Go on a beautiful walk over the highest stone railway bridge in Europe to the church in Sambuca.
- Go wild boar hunting.
- Learn to play local sport *palla elastica* (elastic ball) with the village youths.
- Use TTI's two inflatable boats to play on the Turritecava lake accompanying picnic recommended. Have races. Try to find the Buca del Lago della Turrite Cava (as you sail towards the dam, it is on the left just after the exit of the second road tunnel.
- Go kayaking on the Turritecava. Bring your own canoe.
- Explore the ancient *Vasaio di Motrone* cave in the nearby village of Motrone (see http://www.apuane2007.it/italiano/vasaio/zona_vasaio.php).

12.3 Relaxed activities

- Visit the Pinocchio park, the Garzoni gardens, and the Collodi butterfly house in Collodi. See http://www.pinocchio.it/park.htm.
- The Opera Barga festival is usually on around the same time as the conference (but too early in July for 2014). Ask Mike in advance for tickets and reservations, or see: http://www.operabarga.it/english/.
- Look in the latest issue of Lucca "Grapevine" magazine in English for local cultural activities and concerts etc.. See http://www.luccagrapevine.com/
- Play with the Institute's Victorian Scientific Instrument Collection.
- Spend the afternoon bathing in the outdoor hot pool at the ancient thermal baths of Bagni di Lucca (one of the most fashionable spots in Europe in Lord Byron's time the Switzerland of Tuscany!). Followed by shopping, sightseeing and coffee in the town centre.
- Samantha has two other favourite open-air pools at Gallicano and Barga. These are like little beach resorts where one lazes about on deckchairs and has the occasional dip.
- Watch the night sky through the Institute's astronomical telescope.
- Visit the ancient city of Barga (http://barganews.com) for an afternoon's relaxed sightseeing, shopping and culture.
- Visit the beautiful city of Lucca.

- Visit Castelnuovo di Garfagnana, where you can find Andrea's (the 'Indiana Jones of the Garfagnana') famous Osteria, where all day you can sample fabulous local wines, cheeses and snacks.
- Follow in the footsteps of Michaelangelo, and visit some of the Apuan Alps famous marble quarries.
- Day trip to Florence.
- Drive to the next valley along from ours over a spectacular high mountain road where the eagles live. Visit the Grotta del Vento the Cave of the Winds (http://www.grottadelvento.com). This is the most famous cave system in Tuscany and the visitor will enjoy a spectacular and bizarre landscape of caverns and lakes. Take a pullover as the temperature is a reliable 10 degrees the whole year round. Then head down the valley to visit the *Eremo di Calomini* an ancient monastery built into a high steep cliff.
- Table football and drinking in Fabbriche di Vallico.
- Horse riding at La Fornace.
- Various mild short walks around the Institute.
- Digging the Institute garden and doing little DIY things like restoring the church (I say this merely in hope..).

12.4 Very relaxed activities

- TTI has a high-definition video camera. Make a film of life at one of the world's best conferences.
- Budding archaeologists may use the TTI metal detector bought following a recent spooky event when Evans and Mike were digging a hole in the ground for the satellite dish (I'm really not making this up): MIKE: Hey Evans, watch out for crucifixes when you're digging that hole. This used to be a monastery you know. EVANS (REACHING INTO THE HOLE) What, like this one? (HOLDS UP A THOUSAND YEAR OLD BRONZE CRUCIFIX FROM FIVE FEET DOWN). The crucifix is stored in the monastery in a secret place; please ask to have a look at it.
- Spend all day in the TTI garden relaxing in one of the Institute's three hammocks, drinking wine, snoozing or reading one of the books from the TTI library.
- The Institute has a variety of board games, jigsaws, and similar entertainments together with a number of Victorian books with titles like 'What To Do On Cold Winter Evenings Given That We Haven't Invented Television Yet'.
- Debate physics with the help of the Institute blackboards.
- Listen to one of Mike's lectures inspired by the contents of the TTI Antiquarian Library such as *Richard Burton* and the Source of the Nile (Burton the Victorian explorer and polymath, not the one out of Where Eagles Dare..) or Up The Orinoco with Alexander von Humboldt.
- Spa treatments in the Bagni di Lucca "Thermal resort".
- Mike is translating some chapters of a book on the history of Vallico Sotto. If he's finished it by the time you visit, then walk around the village looking at the buildings and places it describes.

12.5 General

- Volunteer to help clear overgrown local woodland paths (and also to repair some of the ones that collapsed in the great storm of November 2013). Mike can supply gloves and tools..
- The Institute has a wildlife photography notice board. Prizes for the best entries, particularly if you can take a picture of one of the eagles that regular soar above Vallico or of the elusive *marmite*.
- The Towler Institute Exploration Society also has some photographic challenges available see the web site for details.

- Revitalize the economy of Vallico Sotto. It's barely 40 years since 450 people lived here. Now less than 100 do so. Just because modern lazy teenagers want to be fashion models smoking drugs in Milan rather than having a nice healthy outdoor life, the population of rural Italy has been denuded. Let's bring back the time when all the mountain terraces were in production, packs of nice mules helped carry things, teams of volunteers kept paths and bridges open, and everyone knew how to bake chestnut cakes. All serious suggestions gratefully received.
- After the forthcoming Carrington Event (http://en.wikipedia.org/wiki/Solar_storm_of_1859) when all electricity supplies have permanently failed (or some similar apocalyptic event), Vallico Sotto will be the ideal place to shelter from marauding gangs and to begin to rebuild civilization. The recent book 'The Knowledge: how to rebuild our world from scratch, by Lewis Dartnell' explains how to do this. As an exercise, and to help Mike prepare, see if you can figure out how to do some of the essential things that we will need (rig a water-powered electricity supply; find edible plants; make limestone mortar; fortify the monastery against enemy incursion; stuff like that). Buy it here: http://www.amazon.co.uk/Knowledge-How-Rebuild-World-Scratch-ebook/dp/B00H4EM594/ref=sr_1_1?s=books&ie=UTF8&qid=1400500727&sr=1-1

13 FOOD

In general breakfast will be taken in the Institute, lunch in the little bar in Vallico Sotto run by the lovely Monica, and dinner in some local restaurant (on all but one or two evenings outside the village).

In the institute some basic food staples will be provided which participants should feel free to fight over but in general you might like to buy your own food in the village shop run by the lovely and friendly Adelina. However sadly you can't because it closed in late 2007 - much to the consternation of all she relocated to a big new shop down in the main valley in Pian di Coreglia. To replace her, there are two food shops in Fabbriche di Vallico - a five minute drive downhill - and a giant Leclerc supermarket in Gallicano (twenty-five minutes drive). In principle there is also a tiny food shop in Vallico Sopra which seems to open 'on request' by ringing the bell, but I wouldn't rely on it.

To find the Vallico Sotto bar for lunch, go down the tunnel underneath the Doctor's house (the big house opposite the TTI church front door). Then take any path downwards until you get to the Vallico main square - the bar is just underneath that.. You are strongly encouraged to take your lunch here, as normally it doesn't serve food and Monica is doing us a big favour by buying food and preparing it - so we need to make it worth her while. Note you can also get beers, coffees, ice creams and so on here..

Note that people in local shops - or indeed anywhere round here - tend not to speak English, so learning some basic Italian food words before you come will help: pane = bread, formaggio = cheese, prosciutto = ham, pomodori=tomatoes, birrà = beer, vino = wine, caffè = coffee, latte = milk, grazie! = thank you!

You are of course welcome to make use of the Institute's cooking facilities whenever you want. There is a big downstairs kitchen in the main building formerly run by a proper cook - who wrote the *Il Collegio Cookbook* whose recipes you are encouraged to try (it's in the little bookshelf in the kitchen). There are also two kitchens in the adjacent Doctor's house which will be rented for the duration of the conference, and similar facilities in most of the other houses.

On the first evening a simple buffet dinner will be provided. Later in the week the Institute's 16th Century pizza oven may be pressed into service. The rest of the time we will make use of the excellent local restaurants. When very large numbers of people are staying at the Institute, people are encouraged to break up into at least two groups, although many of them - especially Da Sandra - are large enough to handle everyone. Unless told otherwise, Mike will simply assume that you will be coming to each evening meal and will make bookings accordingly (generally a few weeks in advance). These bookings can be changed but please give Mike plenty of notice.

Finally, if you are a vegetarian, you need to be aware that the locals will consider you to be certifiably insane and will feel very sorry that you are unable to enjoy their passion for delicious animal products of all kinds - particularly those made from parts of pigs. Don't worry about this. Following almost a decade of TTI activities, they are now used to us bringing strange foreigners to their restaurants and most are now able to supply vegetarian meals of some kind.

A FEW LOCAL RESTAURANTS

- Mulino Biologico (3280 707037, Fabbriche di Vallico)
- Da Sandra (0583 761289 on the road between Fabbriche di Vallico and Vallico Sotto).
- Il Canapale (0583 761829, Vallico Sopra)
- Al Laghetto (0583 75798, near the lake at the entrance to the Turritecava valley)

- La Rondine (0583 761751 Fabbriche di Vallico, open Fri evening, plus all day Sat/Sun)
- Alto Matanna (0584 776005, Matanna)
- Ristorante Rita e Rinaldo (0583 357728, Focchia)

RESTAURANTS SLIGHTLY FURTHER AFIELD

- Circolo dei Forestieri, Bagni di Lucca
- Antica Trattoria dell'Eremita, Vergemoli
- Il Garfagnino, on the main road near Turritecava.
- Quadrifoglio, on the main road near Calavorno.
- LOTS MORE ASK

SPECIAL RESTAURANTS

- La Buca di Sant'Antonio, Lucca
- La Mora, Ponte a Moriano
- Butterfly, Lucca

See also the TTI Restaurant Guide page on the website.

14 CLEANING ROTA

Guests who have the misfortune to be members of the Cambridge University TCM Group/Imperial College and under the age of 40 are normally press-ganged into trying to keep the Institute clean:

Mike Towler - upstairs kitchen and corridor, church Bartomeu Monserrat-Sanchez - back garden, church Gareth Conduit - upstairs bathroom Jonathan Lloyd-Williams - middle corridor and bathroom, front porch Edgar Engel - downstairs living room, corridor and pantry, front garden Fionn Malone, Sam Azadi - downstairs kitchen

Everyone else please try not to create too much mess for them.

15 CINEMA VALLICO

The requirements of modern science presentations means the Institute church is also the only cinema in the whole of the Apuan Alps - a fact that local people very much enjoy (since the opening presentation of *Cinema Paradiso* in August 2005). During the conference you are welcome to use the projectors and it is expected that movies will be shown on some evenings. The Institute has an extensive DVD library which you are welcome to browse. Feel free also to bring your own movies that you think we might enjoy.

16 NEWS FROM THE TOWLER INSTITUTE

MDT has on occasion written stories about events at the Institute and published them on the local Barga News website. See http://barganews.com and the "News from the Towler Institute" blog (or go to the TTI web site http://vallico.net/tti/tti.html and click on the relevant link in the left-hand column). So far these are mainly about cave explorations and similar adventures. However, Mike doesn't have a monopoly on this. If you wish to contribute your literary efforts then please send your stories about your adventures in Italy to him, and he will ask Keane the Editor to publish them on Barga News.

17 FOOTBALL MATCH: VALLICO SOTTO CONTRO IL MONDO

The thrusting young lads of Vallico Sotto have challenged the Rest of the World - i.e. you - to a game of 5-a-side football on the village pitch. This tradition - which we began many years ago - attracts a large crowd and we always get absolutely caned (even when I have had Brazilians and Spanish people available). Can a small mountain village with less than a hundred inhabitants continue to defy the other 6 billion of us? If you think you can stop them, please volunteer.

VOLUNTEERS

Jasmine Umrigar (age 13)

Everyone else is just afraid..

18 SUMMER SCHOOL

Note that the conference will be followed by a QMC Summer School the following week, taught by Mike Towler and Neil Drummond (with help from Sam Azadi). Schedule and further details available on the web site.

19 MUSIC

After many years of patiently accumulating musical equipment, we have now acquired enough that the TTI church can in principle be used as a professional live music venue. Participants with musical talents are therefore encouraged to demonstrate them..

Our stringed instruments include a basic acoustic guitar, an Epiphone EJ-200CE electro-acoustic guitar, a Line 6 Variax 500 electric guitar, an electric violin, and an antique 17th century violin (currently broken). Note the Variax 500 is a *modelling guitar* (i.e. internal electronics process the sound from individual strings to supposedly model or replicate the sound of specific guitars and other instruments.)

We have two keyboards: (1) a top-of-the-range-in-1995 and still pretty good Technics KN3000 keyboard, which is also our only source of drums, and (2) a beautiful red Nord Piano 2 HA 88 with triple pedal (MDT's pride and joy). This latter is one of the best available stage pianos (really, it's wasted on him) and despite his penchant for playing crude rock and roll songs, it's perfectly capable of having classical music played on it and sounding like a Bösendorfer Imperial Grand (not surprising, because it explicitly samples one, as well as things like Saloon bar honky-tonks). (http://www.nordkeyboards.com/products/nord-piano-2).

There are 3 microphones, 2 of good quality, including a retro-styled Shure Super 55 Deluxe used as a piano floor mike.

There is a Yamaha Stagepas-300 PA system with built-in mixer into which anything electronic in need of amplification may be plugged. The Nord Piano has a couple of Electrovoice ZLX-12P powered loudspeakers which can act as monitors (there is also a wireless monitor system). There is also a Line 6 guitar amplifier (with built-in effects), and an old 1990s Carlsbro keyboard amp (not recommended).

In his role of trainee Jerry Lee Lewis impersonator – limited by severe lack of time to practice – Dr. Towler has been threatening for years to attempt a full-on Fifties rock and roll concert (as detailed on the QMC web site at http://vallico.net/casinoqmc/music/). On payment of a suitable fee (such as a cigarette, which he only smokes during TTI meetings because of the stress), this might even happen - you never know. Anyone who might want to contribute a guitar solo or a backing vocal or even their own song should get in touch beforehand. Dr. López Ríos - who is actually a member of a proper band in Cambridge that plays in front of real people for money - is always happy to strum away on the guitar in the modern style. Dr. Neil Drummond is believed to be able to play the maracas, but we don't have any.

Note as with all musical performances, practice beforehand is always strongly recommended.

20 HEALTH AND SAFETY

We should all recognise that climbing, mountaineering and caving are activities with a danger of personal injury or death. Participants in these activities during their stay at TTI are asked to be aware of and accept these risks and be responsible for their own actions.

The nearest Accident and Emergency Department is 25 minutes away in Barga Hospital (car drivers should satisfy themselves as to its location on Google Maps) - other hospitals are in Lucca (50 minutes) and Castelnuovo di Garfagnana (45 minutes). The Italian emergency telephone number is 112.

Vallico Sotto is a mediaeval village built a thousand years ago on a steep slope with many steps, and naturally there no facilities whatsoever for the disabled; furthermore it seems that the builders of long ago have intentionally set traps designed to kill or injure you. However don't let this put you off; wheelchairs and so on can be manhandled up the hill with you in it if required, and of course we are happy to do this as a way of keeping fit.

TTI is a smoking venue and visitors may smoke as much as they like (ashtrays will be provided).

21 APPENDIX 1: Talk abstracts

The only one I have received this year is from Cyrus:

Cyrus Umrigar

"Semistochastic quantum Monte Carlo -- A hybrid of exact diagonalization and quantum Monte Carlo methods"

This talk will first provide an overview of various zero-temperature QMC methods, discuss their advantages and disadvantages, and the nature of the infamous "Sign Problem". Then the recently developed S emistochastic Quantum Monte Carlo method[1], which combines some of the advantages of Exact Diagonalization with those of the FCIQMC[2,3] method, developed by the Alavi group, will be discussed.

- [1] F. R. Petruzielo, A. A. Holmes, Hitesh J. Changlani, M. P. Nightingale and C. J. Umrigar, Phys. Rev. Lett., 109, 230201, (2012).
- [2] George H Booth, Alex Thom and Ali Alavi, J. Chem. Phys., 131, 054106 (2009).
- [3] Deidre Cleland, George H Booth, and Ali Alavi, J. Chem. Phys., 132, 041103 (2010).

22 FINAL NOTE

Have fun in Vallico Sotto!