1. FINAL EXAM, CIFAR-PITP INTERNATIONAL SUMMER SCHOOL ON NUMERCIAL METHODS IN CONDENSED MATTER 6 JUNE 2008

Duration of the examinaion, 8h30 to 11h30.

The examination counts for 60% of the total. Each of the two homeworks counts for 20%.

There are 49 points. The grade will be pass-fail.

1.1 Short questions with short answers *(29 points)*

a) *(2 points)* In the approach described by M.Ernzerhoff, how can one define the universal functional $F[\rho]$ entering density-functional theory.

Solution: Minimize the kinetic energy plus electron-electron interaction, at fixed density, with respect to all possible wave functions.

$$F[\rho] = \min_{\rho=cst,\psi} [T + V_{e-e}]$$

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b) *(1 point)* What is the physical meaning of "ecut" in the abinit code?

Solution: It is the kinetic energy of the highest energy plane wave for the expansion of the Bloch wave function.

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c) *(2 points)* What is the purpose of the Kohn-Sham procedure in Density Functional Theory?

Solution: *(1 point)* The Kohn-Sham procedure is a convenient basis to represent the density and *(1 point)* it provides a good estimate of the kinetic energy using the usual Schrödinger formula. In addition it provides a non-interacting picture of the many-body problem.

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d) *(2 points)* There is a simple renormalization procedure to solve the Hubbard model on a lattice that consists in diagonalizing a small cluster (block) of

sites exactly, keeping the lowest energy states and using these states to write the Hamiltonian in that smaller new basis. Adjacent clusters are then combined by writing the coupling terms in the new basis and the procedure is iterated. What is the main reason why this procedure fails?

Solution: *(1 point)* The wave functions inside the clusters will be rather short wavelength because of the boundary conditions. *(1 point)* They will be misadapted to expand the true low-energy wave function of the lattice.

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e) *(2 points)* State two important ideas that allow the numerical renormalization group to work properly for the Kondo problem.

Solution: *(1 point)* In the Kondo problem, Wilson assumed s-wave scattering, *(1 point)* adapted the basis in energy space on a logarithmic scale and used rescaling so that all energy scales be considered on the same footing.

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f) *(2 points)* Show simply that the state $|\uparrow\uparrow\rangle+|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle+|\downarrow\downarrow\rangle$ is not entangled.

Solution: *(1 point)* $|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle = |\uparrow\rangle|\uparrow\rangle + |\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle + |\downarrow\rangle|\downarrow\rangle = (|\uparrow\rangle + |\downarrow\rangle)(|\uparrow\rangle + |\downarrow\rangle)$. *(1 point)* Since the state factors into the direct product of states for separate particles, it is not entangled.

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g) *(1 point)* Can Density matrix renormalization group can be viewed as a variational procedure and if so on what type of states?

Solution: *(1 point)* Yes, it can be viewed as a variational procedure on matrix product states.

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h) *(2 points)* In exact diagonalization studies of the Hubbard model, what internal representation of numbers is used to label the states and what is the name of the procedure used to find the state with the lowest energy?

Solution: *(1 point)* The states are labeled with binary numbers. In 32 bit arithmetic for a 16 site problem, 16 bits would be used to represent which sites are occupied by an up spin, and the other 16 bits would be used to represent which sites are occupied by a down spin. *(1 point)* The Lanczos procedure is used to find the lowest energy eigenstate and eigenvalue.

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i) *(3 points)* In the worm algorithm for the Heisenberg model on a lattice, one computes at the same time the Green function and what other quantity? Is it possible to avoid discretization in imaginary time for this case? What other model can we consider with the worm algorithm?

Solution: *(1 point)* One also computes the partition function when I and M are at the same point (joining them is one of the allowed moves). *(1 point)* There is no discretization in imaginary time. *(1 point)* One can also study the Bose-Hubbard model with a similar formalism.

j) *(3 points)* The self-consistent equations for single-site Dynamical Mean-Field Theory can be written as

$$G(\omega) = \sum_{\mathbf{k}} \left(\frac{1}{G_0^{-1}(\mathbf{k},\omega) - \Sigma(\omega)} \right) \tag{1.1}$$

$$\mathcal{G}_0^{-1}(\omega) = G^{-1}(\omega) + \Sigma(\omega). \tag{1.2}$$

Which quantity is used as input for the impurity solver and what is its physical meaning? Which quantity is the output of the impurity solver? Where does the lattice enter the above equations?

Solution: *(1 point)* $\mathcal{G}_0^{-1}(\omega)$ the bath Green function is the input of the impurity solver, *(1 point)* $G(\omega)$ the output. *(1 point)* The lattice enters through the dispersion relation in $G_0^{-1}(\mathbf{k},\omega)$.

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k) *(3 points)* Let

$$Z = e^{-F[J]} = \int d\psi d\psi^\dagger e^{-\left[S(\psi,\psi^\dagger)+JA\right]} \tag{1.3}$$

$$\frac{\delta F[J]}{\delta J} = \langle A \rangle = a \tag{1.4}$$

$$\Gamma[a] = F[J[a]] - aJ[a] \tag{1.5}$$

What is a in Density Functional Theory (DFT) and what is it in Dynamical Mean-Field Theory? If one splits the action into $S = S_0 + S_1$ where S_0 is the action for a non-interacting particle, what plays the role of J_0 in DFT?

Solution: *(1 point)* In DFT, a is the density, in *(1 point)* $DMFT$ it is the local Green function. *(1 point)* J_0 is equal to V_{int} where $V_{ext} + V_{int} = V_{KS}$ with V_{KS} the Kohn-Sham potential.

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l) *(2 points)* If you wanted to study the superfluid stiffness for bosons, what quantum Monte Carlo algorithm would be most suitable and why?

Solution: *(1 point)* The worm algorithm since superfluid stiffness involves winding number, *(1 point)* so it is important to be able to break world lines.

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m) *(2 points)* In the Suzuki-Trotter decomposition for the Hirsch-Fye algorithm, what is the behavior of the systematic error as a function of the discretization time step $\Delta\tau$ and how is it controlled?

Solution: *(1 point)* The error in the end is of order $(\Delta\tau)^2$ and it is controlled by calculating for a few $\Delta\tau$ and *(1 point)* extrapolating to $\Delta\tau = 0$.

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n) *(2 points)* Suppose I want to study an N site Hubbard lattice using the hybridization expansion with continuous-time quantum Monte Carlo method. How does the size of the problem scale with N.

Solution: *(1 point)* One needs the exact solution on the cluster, *(1 point)* so the problem will scale like 4^N for the Hubbard model where each site in the grand-canonical ensemble can be empty, singly occupied or doubly occupied.

1.2 Metropolis algorithm *(4 points)*

Let $P(x)$ be the probability for a spin configuration x and $w(x \to y)$ the transition probability in a Markov chain that allows transition between these two states. Using the Metropolis algorithm, fill in the following table and show that detailed balance is satisfied.

	$w(x \to y)$	$w(y \to x)$
$P(x) > P(y)$		
$P(x) < P(y)$		

Solution: *(2 points)*

	$w(x \to y)$	$w(y \to x)$
$P(x) > P(y)$	$P(y)/P(x)$	1
$P(x) < P(y)$	1	$P(x)/P(y)$

(2 points) and clearly for the first row

$$P(x)\, w(x \to y) = P(x)\, P(y)/P(x) = P(y) = P(y)\, w(y \to x) \tag{1.6}$$

while for the second row

$$P(x)\, w(x \to y) = P(x) = P(y)\, w(y \to x) = P(y)\, P(x)/P(y) \tag{1.7}$$

1.3 Variance in a Monte Carlo calculation *(10 points)*

a) *(6 points)* If the variance of a random variable is $\sigma_A^2 = \langle A^2 \rangle - \langle A \rangle^2$, show that if A_i are samples of that random variable, then $\frac{1}{N}\sum_i^N A_i$ has a variance equal to σ_A^2/N only if the samples are statistically independent.

b) *(4 points)* How do the subroutines in ALPS check for statistical independence? (Do not give too many details, be brief).

Solution: a) *(1 point)* Let $\langle A\rangle$ be the true expectation value of the observable and A_i the result of the i^{th} measurement. The mean is estimated from $\sum_i^N A_i$. The expectation of A_i, is equal to $\langle A\rangle$ so

$$\left\langle \frac{1}{N}\sum_i^N A_i \right\rangle = \langle A\rangle \,. \tag{1.8}$$

(3 points) On the other hand, $\sum_i^N A_i$ is a random variable whose variance can be calculated for any realization. The expected value of that variance is

$$\begin{aligned}
\sigma^2 &= \left\langle \left[\left(\frac{1}{N}\sum_i^N A_i \right) - \langle A\rangle \right]^2 \right\rangle = \frac{1}{N^2}\left(\sum_i^N \sum_j^N \langle A_i A_j\rangle \right) - \frac{2}{N}\sum_i^N \langle A_i\rangle \langle A\rangle + \langle A\rangle^2 \\
&= \frac{1}{N^2}\left(\sum_i^N \sum_j^N \langle A_i A_j\rangle \right) - \langle A\rangle^2 \qquad (1.9) \\
&= \frac{1}{N^2}\left(\sum_i^N \sum_j^N \left(\langle A_i A_j\rangle - \langle A\rangle^2 \right) \right) \qquad (1.10) \\
&= \frac{1}{N^2}\left(\sum_i^N \left(\langle A_i^2\rangle - \langle A\rangle^2 \right) \right) + \frac{1}{N^2}\sum_i^N \sum_{i\neq j}^N \left(\langle A_i A_j\rangle - \langle A\rangle^2 \right) \qquad (1.11)
\end{aligned}$$

(1 point) The last term is related to correlations. If $\langle A_i A_j\rangle = \langle A_i\rangle \langle A_j\rangle$, then the last term vanishes and we have σ_A^2/N for the variance. Generally, the last term will not vanish.

$$\begin{aligned}
\frac{1}{N^2}\sum_i^N \sum_{i\neq j}^N \left(\langle A_i A_j\rangle - \langle A\rangle^2 \right) &= \frac{2}{N^2}\sum_i^N \sum_{i<j}^N \left(\langle A_i A_j\rangle - \langle A\rangle^2 \right) \\
&\simeq \frac{2}{N}\sum_{j=2}^{\infty} \left(\langle A_1 A_j\rangle - \langle A\rangle^2 \right) \\
&= \frac{2\tau_A \sigma_A^2}{N} \qquad (1.12)
\end{aligned}$$

(1 point) where the last two equations define the correlation time τ_A.*In* the presence of correlations then

$$\sigma^2 = \frac{\sigma_A^2\,(1+2\tau_A)}{N} \tag{1.13}$$

b) *(4 points)* In ALPS, N data are binned by groups of 2^n measurements. Each group becomes what we now call a measurement. In the presence of correlations, if we estimate σ^2 as if the measurements were independent ($\tau_A = 0$) we will get an underestimate since the true variance will be given by the result above. With σ_n^2 the variance for bins of 2^n measurements, ALPS outputs $\sigma_n^2/\left(N/2^n\right)$ as a variance. The best estimate of the variance is obtained from the latter in the limit where it becomes independent of n.

1.4 Reduced density matrix and Density Matrix Renormalization Group *(4 points)*

a) *(3 points)* If $|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle$ is a wave function that describes a system of interest $|i\rangle$ and a reservoir $|j\rangle$. What is the reduced density matrix that can be used to describe only the subsystem i?

b) *(1 point)* If there are l states in subsystem i, how does one reduce the size of the basis to m states in DMRG?

Solution: a) *(1 point)* The full density matrix is given by

$$\rho = |\psi\rangle \langle\psi| . \tag{1.14}$$

(1 point) To compute the expectation value of a quantity defined in the system of interest, we need

$$\mathrm{Tr}\rho O_i \tag{1.15}$$

where O_i is defined only in the system of interest i. Since the trace can be performed in two steps,

$$\mathrm{Tr}\rho O_i = \mathrm{Tr}_i \mathrm{Tr}_j \rho O_i$$

(1 point) one can compute the expectation value of any operator O_i from the reduced density matrix

$$\mathrm{Tr}_j \rho = \sum_j \psi_{ij} |i\rangle \langle i'| \psi^*_{i'j}. \tag{1.16}$$

b) *(1 point)* One diagonalizes the density matrix and keeps the lowest m states.

1.5 Hirsch-Hubbard-Stratonovich transformation *(2 points)*

In determinantal Quantum Monte Carlo for the Hubbard model, one does the Trotter decomposition and then transforms the interaction between spin up and spin down into spins interacting with a field using the following transformation at each space-time point

$$e^{-\Delta\tau U\left(n_\uparrow n_\downarrow - \frac{1}{2}(n_\uparrow + n_\downarrow)\right)} = \frac{1}{2} \sum_{s=\pm 1} e^{\alpha s (n_\uparrow - n_\downarrow)}. \tag{1.17}$$

Prove that this is satisfied if $\cosh\alpha = e^{\Delta\tau U/2}$.

Solution: *(2 points)* There are only four states on which these operators act, so it suffices to proceed by enumeration

$n_\uparrow$	$n_\downarrow$	$e^{-\Delta\tau U\left(n_\uparrow n_\downarrow - \frac{1}{2}(n_\uparrow + n_\downarrow)\right)}$	$\frac{1}{2}\sum_{s=\pm 1} e^{\alpha s (n_\uparrow - n_\downarrow)}$
0	0	1	1
1	0	$e^{\Delta\tau U/2}$	$\cosh\alpha$
0	1	$e^{\Delta\tau U/2}$	$\cosh\alpha$
1	1	1	1

The end of the examination