Theory and Computation of High-Temperature Superconductors

3 hours · 100 points

Answer all questions. This is a closed-book test; data and formulas are on the last page. Parts I and II need no justification. In Part III, show your reasoning: most of the credit is for the physics. Use extra sheets if needed. Set $\hbar = k_B = 1$ and the lattice constant to 1, and use Gaussian units ($4\pi\varepsilon_0 = 1$), unless stated otherwise.

(12 points) Part I: True/false questions

Mark each statement True (T) or False (F). Each question is worth 2 points.

1. ( ) For a single electron, such as the hydrogen atom, the local density approximation (LDA) to the exchange–correlation energy exactly cancels the Hartree energy.
2. ( ) For the Hubbard model on two sites with two electrons and $U \gg t$, the spin singlet lies below the triplet by $2t^2/U$.
3. ( ) A strictly two-dimensional Heisenberg antiferromagnet with isotropic, short-range exchange has no Néel order at any $T > 0$.
4. ( ) A few percent of non-magnetic impurities strongly suppress T_c of a d-wave superconductor.
5. ( ) In a Fermi liquid, the quasiparticle weight Z can exceed 1.
6. ( ) Determinant quantum Monte Carlo (DQMC) of the repulsive Hubbard model at half filling, with the standard spin-channel Hubbard–Stratonovich decoupling, has no sign problem on a bipartite lattice with nearest-neighbour hopping only.

(18 points) Part II: Fill in the blanks

Each question is worth 3 points.

7. For the three-dimensional uniform electron gas, on which the LDA is built, the exchange energy per electron scales with the density as $\varepsilon_x \propto -n^p$, with $p =$ _____.
8. Define the exchange–correlation hole as $n_{\mathrm{xc}}(\boldsymbol{r}, \boldsymbol{r}') = n_2(\boldsymbol{r}, \boldsymbol{r}')/n(\boldsymbol{r}) - n(\boldsymbol{r}')$, where n_2 is the pair density. Then $\int n_{\mathrm{xc}}(\boldsymbol{r}, \boldsymbol{r}')d^3r' =$ _____.
9. In Hartree–Fock theory, the paramagnetic metal of the Hubbard model becomes ferromagnetic when $U\rho(E_F) >$ _____, where $\rho(E_F)$ is the density of states per spin per site at the Fermi level.
10. The Néel state of a 3D Heisenberg antiferromagnet breaks SU(2) spin symmetry down to U(1). The number of linearly dispersing Goldstone modes is _____.
11. At hole doping p (electron density $1 - p$ per site), Luttinger's theorem says the hole-like Fermi surface of a paramagnetic single-band metal around (π, π) encloses a fraction _____ of the Brillouin zone.
12. In a three-dimensional Fermi liquid, the quasiparticle scattering rate at the Fermi level grows with temperature as T^α, with $\alpha =$ _____.

(70 points) Part III: Problems. Show all your work and justify your answers.

13. (14 points) Density functional theory (DFT). Kohn–Sham (KS) DFT is the usual starting point for a real material. Take La_2CuO_4 as the example. It contains CuO_2 planes with one hole per Cu ($3d^9$) in the $d_{x^2-y^2}$ orbital, hybridised with O $2p_\sigma$. It is an antiferromagnetic insulator with $T_N = 325$ K and an optical gap of about 2 eV.

(a) (4 pts) Write the KS equations and the effective potential, and say which part the local density approximation (LDA) approximates. What does exact DFT guarantee, and what does it not guarantee about the KS eigenvalues? Why do LDA bands nevertheless agree well with photoemission for high-density simple metals such as Al?

(b) (5 pts) A plane-wave code keeps all plane waves with kinetic energy below a cutoff E_{cut}. Show that the number of basis functions is $N_{\mathrm{pw}} \propto \Omega E_{\mathrm{cut}}^{3/2}$, where Ω is the unit-cell volume. Why do O $2p$ and Cu $3d$ states need a high cutoff, and what do pseudopotentials do? Why does a metal need a denser $\boldsymbol{k}$-point mesh than an insulator? Smearing the occupations speeds up convergence; what does it cost?

(c) (5 pts) Explain why spin-unpolarised LDA predicts La_2CuO_4 to be a metal. DFT+U adds a Hubbard-like energy $E_U = (U/2)\sum_{m\sigma} n_{m\sigma}(1 - n_{m\sigma})$ for the occupations $n_{m\sigma}$ of the Cu d orbitals m with spin σ. Show that the orbital potential is $V_{m\sigma} = U(1/2 - n_{m\sigma})$ and find the splitting between a filled and an empty orbital. Why does DFT+U open a gap only if spin-symmetry-breaking (magnetic) order, such as antiferromagnetism, is allowed? What does this tell you about the method?

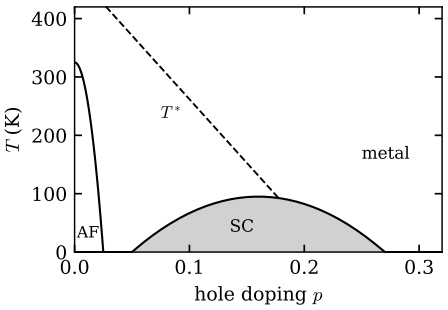
14. (14 points) The Hubbard model and its mean-field theory. Spectroscopy on La_2CuO_4 gives a Cu–O charge-transfer energy $\Delta_{pd} \approx 3$ eV (cost to move a hole from Cu to O) and an on-site Cu repulsion $U_{dd} \approx 8$ eV. The low-energy model is the half-filled Hubbard model on the square lattice, $H = \sum_{\boldsymbol{k}\sigma} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma} + U \sum_i \big(n_{i\uparrow} - 1/2\big)\big(n_{i\downarrow} - 1/2\big)$, with $\varepsilon_{\boldsymbol{k}} = -2t\big(\cos k_x + \cos k_y\big)$. The $-1/2$ shifts put the chemical potential at $\mu = 0$. Let $\boldsymbol{Q} = (\pi, \pi)$, and $\sigma = +1(-1)$ for spin up (down).

(a) (3 pts) In the Zaanen–Sawatzky–Allen classification, is La_2CuO_4 a Mott–Hubbard or a charge-transfer insulator? On which orbitals do doped holes go? Explain briefly why a one-band Hubbard model can still describe the low-energy physics (Zhang–Rice singlet), and which energy plays the role of U.

(b) (5 pts) In the Hartree decoupling, take $\langle n_{i\sigma} \rangle = 1/2 + \sigma e^{i\boldsymbol{Q}\cdot\boldsymbol{r}_i} m/2$ (Néel order with staggered moment m). Show that the mean field couples $\boldsymbol{k}$ to $\boldsymbol{k} + \boldsymbol{Q}$ with amplitude $\Delta = Um/2$. Use $\varepsilon_{\boldsymbol{k}+\boldsymbol{Q}} = -\varepsilon_{\boldsymbol{k}}$ to find the quasiparticle bands $\pm E_{\boldsymbol{k}}$ (with $E_{\boldsymbol{k}} \geq 0$) and the gap.

(c) (6 pts) Self-consistency reads $1/U = (1/N) \sum_{\boldsymbol{k}} \tanh(E_{\boldsymbol{k}}/2T)/2E_{\boldsymbol{k}}$, with the sum over the full Brillouin zone. (i) For $t \to 0$, show $m = \tanh(Um/4T)$; find the gap at $T = 0$ and the mean-field Néel temperature. (ii) At $T = 0$ and small U, show that a solution exists for every $U > 0$. Near $\varepsilon = 0$ the square-lattice density of states per spin has a van Hove singularity, $\rho(\varepsilon) \approx \ln(16t/\,|\varepsilon|)/(2\pi^2 t)$; use it to find how Δ depends on U. (iii) For $t = 0.35$ eV, $U = 3.8$ eV, estimate the Hartree–Fock T_N from (i). Compare it with $J = 4t^2/U$ and with the measured 325 K. Which physical distinction does Hartree–Fock miss?

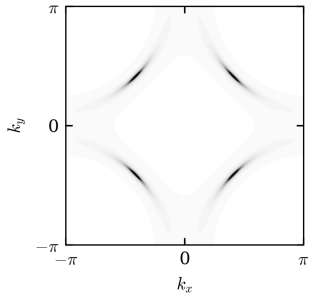
15. (14 points) Superconductivity and pairing symmetry. The figure shows the generic phase diagram of hole-doped cuprates: antiferromagnet (AF), superconducting dome (SC) and pseudogap temperature T^*, below which a partial gap appears in the normal state. The linearised gap equation is $\Delta_{\boldsymbol{k}} = -(1/N)\sum_{\boldsymbol{k}'} V_{\boldsymbol{k}\boldsymbol{k}'} F_{\boldsymbol{k}'} \Delta_{\boldsymbol{k}'}$ with $F_{\boldsymbol{k}} = \tanh(\xi_{\boldsymbol{k}}/2T)/2\xi_{\boldsymbol{k}} > 0$.



(a) (4 pts) Take an attraction $V_{\boldsymbol{k}\boldsymbol{k}'} = -V$ ($V > 0$) for states within ω_D of E_F, and a constant density of states per spin ρ. Show that at $T = 0$ the full gap equation gives $\Delta_0 \approx 2\omega_D e^{-1/\rho V}$ in weak coupling ($\rho V \ll 1$). Why can no finite order of perturbation theory in V produce this result? What does it predict for the isotope effect?

(b) (5 pts) Near the antiferromagnet, spin fluctuations give a repulsive interaction $V_{\boldsymbol{k}\boldsymbol{k}'} > 0$ peaked at $\boldsymbol{k} - \boldsymbol{k}' \approx \boldsymbol{Q} = (\pi, \pi)$. Show that a constant gap has no solution, while a gap with $\Delta_{\boldsymbol{k}+\boldsymbol{Q}} = -\Delta_{\boldsymbol{k}}$ can have one. Check that $\Delta_{\boldsymbol{k}} \propto \cos k_x - \cos k_y$ has this property. On the square-lattice cuprate Fermi surface near half filling, where is this gap largest, and where does it vanish? The image below shows the angle-resolved photoemission (ARPES) intensity at E_F in the superconducting state, at low temperature; darker means higher intensity. Explain its pattern.

(c) (5 pts) An underdoped sample has a maximum gap $\Delta_0 = 40$ meV but a 2D phase stiffness (the energy cost of twisting the superconducting phase) of only $\rho_s(0) = 5$ meV per layer. Estimate the mean-field T_c using $2\Delta_0/T_c = 4.28$ (d wave). Estimate an upper bound from the Berezinskii–Kosterlitz–Thouless (BKT) condition $T_{\mathrm{BKT}} = (\pi/2)\rho_s(T_{\mathrm{BKT}})$. Which sets T_c? Interpret the range between the two, and relate it to $T_c \propto \rho_s(0)$ in underdoped cuprates (Uemura). Where is this range on the phase diagram?



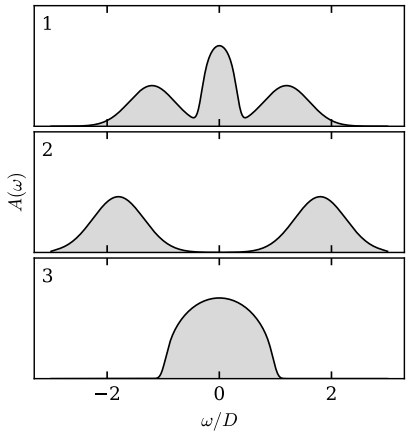
16. (14 points) Dynamical mean-field theory (DMFT). DMFT maps the Hubbard model onto a single impurity site coupled to a self-consistent bath of non-interacting electrons. The self-energy is taken to be local, $\Sigma(\boldsymbol{k}, i\omega_n) \to \Sigma(i\omega_n)$.

(a) (4 pts) Write the DMFT self-consistency loop: how the local Green's function is obtained from Σ, how the Weiss field $\mathcal{G}_0$ (the impurity's Green's function without its own interaction, which encodes the bath) is defined, what the impurity solver computes, and how Σ is updated. Which step is expensive? In which limit is DMFT exact, and how must t scale in that limit? What exactly stays finite?

(b) (4 pts) Consider the paramagnetic Hubbard model on a Bethe lattice of half-bandwidth D at $T = 0$. Here the interaction is written as $U \sum_i n_{i\uparrow} n_{i\downarrow}$, without the shifts of Problem 14, so half filling means $\mu = U/2$. Near $\omega = 0$ the converged self-energy has $\mathrm{Re}\,\Sigma(\omega) \approx U/2 - 1.5\omega$. Find the quasiparticle weight Z and m^*/m. The figure shows the local spectral function $A(\omega)$ versus ω/D at three values of U, in random order. Order them by U and identify the quasiparticle peak and the Hubbard bands. Why is $A(0)$ the same in panels 1 and 3? Where does the weight go as U grows?

(c) (3 pts) Quantum Monte Carlo (QMC) impurity solvers give $G(i\omega_n)$ on the imaginary (Matsubara) axis. Real-frequency spectra require inverting $G(i\omega_n) = \int d\omega A(\omega)/(i\omega_n - \omega)$. Why is this ill-posed? Name one standard remedy and its main weakness.

(d) (3 pts) Why can single-site DMFT describe the Mott insulator but not d-wave superconductivity, or a pseudogap that opens only near $(\pi, 0)$? What is the smallest cluster that can hold a d-wave order parameter, and what is the price of larger clusters?



17. (14 points) Numerical methods for correlated electrons. Is the ground state of the Hubbard model at hole doping $p = 1/8$, $U = 8t$ striped (charge and spin density modulated along one direction) or a uniform d-wave superconductor? The competing states differ in energy by only 0.001–0.01t per site.

(a) (4 pts) Exact diagonalisation (ED) stores the full many-body state vector. Each Hubbard site has 4 states. Find the dimension of the half-filled, $S^z = 0$ sector for $N = 16$ and $N = 20$ sites, and the memory of one vector of real double-precision (8-byte) numbers. Compare with the spin-1/2 Heisenberg model on the same clusters. Why can ED not decide the stripe question?

(b) (4 pts) In determinant quantum Monte Carlo (DQMC), the cost per sweep is $\propto \beta N^3$ and the average sign is $\langle s \rangle \approx e^{-\beta N \Delta f}$, with $\Delta f > 0$. How many samples are needed for a fixed statistical error? A run on N sites has $\langle s \rangle = 0.1$; by what factor does the total cost grow if N is doubled at the same β? Why is this qualitatively worse than the N^3 factor?

(c) (4 pts) A matrix-product state (MPS) with bond dimension χ can carry entanglement entropy $S \leq \ln \chi$ across a cut. The density-matrix renormalisation group (DMRG) optimises an MPS at cost $\propto \chi^3$. Explain why the cost grows exponentially with the width W of a cylinder. DMRG energies per site on a width-6 cylinder are $-0.7600t$ at truncation error 2×10^{-5} and $-0.7630t$ at 10^{-5} (the truncation error is the discarded weight of the reduced density matrix). Extrapolate linearly to zero truncation error, and compare the size of the extrapolation with the energy differences above. Why can the finite width bias the stripe question?

(d) (2 pts) Benchmarks of this ground state pair DMRG with constrained-path auxiliary-field QMC (AFQMC). AFQMC avoids the sign problem by discarding random walkers whose overlap with a trial wavefunction would change sign. What does this constraint cost? Why does agreement between DMRG and AFQMC carry more weight than a smaller error bar from either one?

Data and formulas

- La_2CuO_4: $T_N = 325$ K, optical gap ≈ 2 eV. One-band Hubbard parameters: $t \approx 0.35$ eV, $U \approx 3.8$ eV $\approx 11t$, giving $J \approx 130$ meV. Units: 1 eV = 11605 K.
- Large-U Hubbard model at half filling: Heisenberg model with $J = 4t^2/U$.
- Gap equation: $\Delta_{\boldsymbol{k}} = -(1/N)\sum_{\boldsymbol{k}'} V_{\boldsymbol{k}\boldsymbol{k}'}\Delta_{\boldsymbol{k}'}\tanh(E_{\boldsymbol{k}'}/2T)/2E_{\boldsymbol{k}'}$, $E_{\boldsymbol{k}} = \sqrt{\xi_{\boldsymbol{k}}^2 + |\Delta_{\boldsymbol{k}}|^2}$. Weak coupling: $2\Delta_0/T_c = 3.53$ (s wave), 4.28 (d wave, maximum gap). $\operatorname{arsinh} x = \ln\left(x + \sqrt{x^2+1}\right)$.
- BKT: $T_{\mathrm{BKT}} = (\pi/2)\rho_s(T_{\mathrm{BKT}})$, for $F = (\rho_s/2)\int|\nabla\theta|^2\, d^2r$.
- Green's function: $G(\boldsymbol{k}, i\omega_n) = [i\omega_n + \mu - \varepsilon_{\boldsymbol{k}} - \Sigma(\boldsymbol{k}, i\omega_n)]^{-1}$, $\omega_n = (2n+1)\pi T$. Quasiparticle weight $Z = [1 - \partial_\omega \operatorname{Re}\Sigma(\omega)]^{-1}_{\omega=0}$; for a local Σ, $m^*/m = 1/Z$.
- $\binom{16}{8} = 12870$, $\binom{20}{10} = 184756$.