Faculty of Physics, Lomonosov Moscow State University

Advanced Quantum Field Theory: Modern Applications in HEP, Astro & Cond-Mat
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Handout (Fall 2020 term) – FINAL VERSION

1. *[Bloch's theorem]* From quantum mechanics we know a theorem claiming that two commuting *Hermitian* operators possess a complete joint eigensystem in the Hilbert space. Using this theorem as a starting point, demonstrate existence of a complete orthonormal system of eigenfunctions of a (*non-Hermitian*) translation operator $\hat{T}_{\boldsymbol{d}} \equiv e^{\boldsymbol{d}\cdot\boldsymbol{\nabla}}$ that are also eigenfunctions of the Hamiltonian $\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\boldsymbol{x})$, $V(\boldsymbol{x}+\boldsymbol{d}) = V(\boldsymbol{x})$. *Note: the spectrum of $\hat{H}$ may well be degenerate.*

2. Trans-polyacetylene $(\mathrm{CH})_n$ is a linear polymer, which is known to develop a conjugated (delocalized) orbital from one p_z orbital per each of the carbon atoms. It is also known to *dimerize*, i.e., to exist in the form with alternating 'single' (weaker) and 'double' (stronger) bonds $(-\mathrm{CH}=\mathrm{CH}-)_n$. From the tight-binding standpoint, such a system is described by the Su–Schrieffer–Heeger (SSH) model with the Hamiltonian

$$\hat{H} = \sum_{n=-\infty}^{\infty} \sum_{\sigma=\pm} \left\{ u \hat{c}^\dagger_{2n,\sigma} \hat{c}_{2n+1,\sigma} + v \hat{c}^\dagger_{2n,\sigma} \hat{c}_{2n-1,\sigma} \right\} + \text{h.c.}$$

   featuring 'single-bond' and 'double-bond' hopping integrals $u, v \in \mathbb{C}$ and two possible spin projections σ. Find the energy dispersion relation $\varepsilon(k)$ for this TB model, the energy gap, and the effective mass at the lowest point of the conduction band ($\varepsilon > 0$). *Note: mind the unit cell first! Also note that the system is at half-filling so just half the total number of states are occupied!*

3. Find the Brillouin zone for a $2D$ honeycomb lattice (lattice parameter d) and, by translating certain pieces of it by reciprocal-lattice vectors, transform it into a hexagon. After such a visual rearrangement, the Brillouin zone explicitly respects the rotational symmetry of the honeycomb lattice.

4. Express a Hartree–Fock two-electron ground-state wave function for a helium atom ($Z = N = 2, \boldsymbol{S}^2 = 0$) in terms of a single unknown scalar function. Approximating this function as (a) a hydrogenlike $1s$ orbital, (b) a linear combination of a reasonable number of hydrogenlike orbitals, find the HF ground-state energies. Also find the RMS charge radii $\sqrt{\frac{1}{2}\int n(\boldsymbol{x})\boldsymbol{x}^2 \mathrm{d}^3x}$, where $n(\boldsymbol{x})$ is the total charge density of the two electrons, in units of e. *Note: numerical calculations are not forbidden here.*

5. Find the density profile $n(r)$ for a neutral atom with the nucleus charge $-Ze$ using the Thomas–Fermi equation (let us assume that this solution is spherically symmetric). Namely, (i) find the form of the $r \to \infty$ and $r \to 0$ asymptotics of the 'internal potential' $v_{\mathrm{i}}(r)$ and the density, (ii) find the chemical potential, (iii) place appropriate boundary conditions at $r \to \infty$ and the $r \to 0$ and solve this boundary-value problem numerically, e.g., using the shooting method.

6. *[Low-density LDA]* Find the leading coefficient g_0 in the exchange-correlation energy of a dilute homogeneous electron gas of density n,

$$\epsilon_{\mathrm{xc}} = g_0 n^{1/3} + \mathcal{O}(n^{1/2}), \qquad n \to 0.$$

   Hint: Estimate the ground-state energy $E[n] = \langle \mathrm{gnd} | \hat{H} | \mathrm{gnd} \rangle$ of such a gas from QM perturbation theory in the Coulomb interaction and then extract the exchange-correlation energy from $E[n]$ using DFT definitions.

7. *[Friedel oscillations]* A linear semi-infinite chain of atoms is described by a tight-binding model at half-filling with nearest-neighbor transfer integrals equal to $-t$. Calculate the average on-site electron numbers $n(j) = \sum_\sigma \langle \hat{c}^\dagger_{j\sigma} \hat{c}_{j\sigma} \rangle$ as a function of the site number $j = 1, 2, 3, \ldots$. Compare your result with the 2D case of a half-plane with a square lattice.

8. Show that for a lattice with the primitive cell containing only one lattice site, the electron Green's function in the tight-binding model is

$$\begin{aligned} G_{\sigma\sigma'}(\boldsymbol{x}, \boldsymbol{y}, t) &\equiv -\mathrm{i} \langle \mathrm{FS} | \, \mathrm{T} \hat{c}_\sigma(\boldsymbol{x}, t) \hat{c}^\dagger_{\sigma'}(\boldsymbol{y}, 0) \, | \mathrm{FS} \rangle \\ &= \delta_{\sigma,\sigma'} \int\limits_{-\infty}^{+\infty} \frac{e^{-\mathrm{i}\omega t} \mathrm{d}\omega}{2\pi} \sum_{\boldsymbol{k} \in \mathrm{BZ}} \frac{e^{\mathrm{i}\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{y})}}{\Omega} \left\{ \frac{\vartheta(\epsilon_{\boldsymbol{k}} - \varepsilon_\mathrm{F})}{\omega - \epsilon_{\boldsymbol{k}} + \mathrm{i}0} + \frac{\vartheta(\varepsilon_\mathrm{F} - \epsilon_{-\boldsymbol{k}})}{\omega - \epsilon_{-\boldsymbol{k}} - \mathrm{i}0} \right\}, \end{aligned}$$

where Ω is the total number of the lattice sites (= the number of points in the Brillouin zone), $\epsilon_{\boldsymbol{k}}$ is the spectrum of 1-particle energies, and ε_F is the Fermi energy. *Note:* prove and then use the identity on the Heaviside ϑ function

$$\vartheta(t) e^{-\mathrm{i}\Omega t} = \int\limits_{-\infty}^{+\infty} \frac{\mathrm{i}\mathrm{d}\omega}{2\pi} \frac{e^{-\mathrm{i}\omega t}}{\omega - \Omega + \mathrm{i}0}.$$

9. Let us look at a hydrogen H_2 molecule from a Hubbard model perspective

$$\hat{H} = -t(d) \sum_{\sigma=\uparrow,\downarrow} \left\{ \hat{c}^\dagger_{1\sigma} \hat{c}_{2\sigma} + \hat{c}^\dagger_{2\sigma} \hat{c}_{1\sigma} \right\} + U \sum_{i=1,2} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \qquad N = 2.$$

Here, we have only two sites $i = 1, 2$ and four creation operators $\hat{c}^\dagger_{i\sigma}$; the transfer integral strongly depends on the orbital overlap, so it is assumed to depend on the distance d between the two nuclei. Using the fact that the four operators $\hat{\boldsymbol{S}}^2 = (\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2$, $\hat{S}_z = \hat{S}_{1z} + \hat{S}_{2z}$, $\hat{P}$, and $\hat{N} = \sum_{i,\sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{i\sigma}$ commute with each other and with $\hat{H}$, find the energies and wave functions of triplet $S = 1$ and singlet $S = 0$ states of the molecule. The parity operator simply exchanges the two sites, $\hat{P}^{-1} \hat{c}_{i\sigma} \hat{P} := \hat{c}_{3-i,\sigma}$. Compare your results with the tight-binding ($U = 0$) case.

10. Find the divergent part of the density of states for a tight-binding model on a 2D square lattice with all NN hopping integrals equal to t

$$\rho(\epsilon) = \frac{N}{\pi^2 t} \log \frac{t}{|\epsilon|} + \mathcal{O}(1), \quad \epsilon \to 0 \qquad \text{(lattice units, } d = 1\text{)}.$$

This *Van Hove singularity* takes place exactly at the Fermi surface in the case of half-filling.

11. Apply a Bogolyubov transformation to the mean-field BCS Hamiltonian

$$\begin{aligned} \hat{H} - \mu \hat{N} &= \sum_{\boldsymbol{k}\sigma} (\epsilon_{\boldsymbol{k}} - \mu) \hat{c}^\dagger_{\boldsymbol{k}\sigma} \hat{c}_{\boldsymbol{k}\sigma} - \sum_{\boldsymbol{k}} \left\{ \Delta^* \hat{c}_{-\boldsymbol{k}\downarrow} \hat{c}_{\boldsymbol{k}\uparrow} + \mathrm{h.c.} \right\} + \frac{V}{a^3 U_0} |\Delta|^2, \\ \hat{c}_{\boldsymbol{k}\uparrow} &= u^*_{\boldsymbol{k}} \hat{\gamma}_{\boldsymbol{k}\uparrow} + v_{\boldsymbol{k}} \hat{\gamma}^\dagger_{-\boldsymbol{k}\downarrow}, \\ \hat{c}^\dagger_{-\boldsymbol{k}\downarrow} &= -v^*_{\boldsymbol{k}} \hat{\gamma}_{\boldsymbol{k}\uparrow} + u_{\boldsymbol{k}} \hat{\gamma}^\dagger_{-\boldsymbol{k}\downarrow}, \end{aligned}$$

where $|u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 = 1$. By finding the appropriate $u_{\boldsymbol{k}}, v_{\boldsymbol{k}}$ coefficients, eliminate the particle number violating terms and find the quasiparticle energies as a function of Δ.

12. Consider a graphene sheet with a small *Kekulé distortion* of the lattice, which corresponds to

$$\begin{aligned} \hat{H} &= -\sum_{\boldsymbol{x} \in A} \sum_{j=1,2,3} (t + \Delta t_j(\boldsymbol{x})) \hat{b}^\dagger_\sigma(\boldsymbol{x} + \boldsymbol{\delta}_j) \hat{a}_\sigma(\boldsymbol{x}) + \mathrm{h.c.}, \\ \Delta t_j(\boldsymbol{x}) &= \frac{\kappa}{3} \left\{ e^{\mathrm{i}(\boldsymbol{Q} \cdot \boldsymbol{x} + \boldsymbol{k}_+ \cdot \boldsymbol{\delta}_j)} + \mathrm{c.c.} \right\} \to 0, \end{aligned}$$

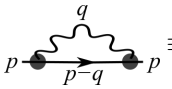
where $\boldsymbol{Q} \equiv \boldsymbol{k}_+ - \boldsymbol{k}_-$ is the vector connecting the two Fermi points of pristine graphene. Find the effective Dirac equation describing quasiparticles near the Fermi surface that results from such a perturbation (N.B.: it will mix the two Fermi points!).

13. Find the one-particle eigenstates and their energies for the π-band electrons in graphene in the external magnetic field $\boldsymbol{B} = B\boldsymbol{e}_z$ orthogonal to the graphene plane (neglecting the Zeeman interaction $\sigma\mu_{\rm B}B$). Use the potential $\boldsymbol{A}(\boldsymbol{x}) = eBx\boldsymbol{e}_y$.

14. In the $\xi = 1$ gauge, integrate out the photon field A_μ in the partition function $Z[\xi_\sigma, \bar{\xi}_\sigma]$ for the π electrons in graphene ($\xi_\sigma(x), \bar{\xi}_\sigma(x)$ are the sources conjugate to the spinor fields $\bar{\Psi}_\sigma(x), \Psi_\sigma(x)$, respectively). As a result, find the effective action for the interacting graphene and resort to its nonrelativistic limit

$$\begin{aligned} S_{\rm eff}[\Psi_\sigma, \bar{\Psi}_\sigma] &= \int d^3x \bar{\Psi}_\sigma(x)\, \mathrm{i}(\gamma^0\partial_0 + v_{\rm F}\boldsymbol{\gamma}\cdot\boldsymbol{\nabla})\, \Psi_\sigma(x) \\ &- \frac{e^2}{8\pi}\int \mathrm{d}t\mathrm{d}^2x\mathrm{d}^2y \frac{\bar{\Psi}_\sigma(\boldsymbol{x})\gamma^0\Psi_\sigma(\boldsymbol{x})\ \bar{\Psi}_\varsigma(\boldsymbol{y})\gamma^0\Psi_\varsigma(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}. \end{aligned} \tag{1}$$

15. From the above action (1), find the one-loop self-energy $\Sigma(p)$ of a quasiparticle (electron/hole) in graphene. Namely, use a momentum cutoff $|\boldsymbol{q}| \leq \Lambda \to +\infty$ and demonstrate that



$$\equiv \Sigma(p) = -\frac{\mathrm{i}e^2}{32\pi}\boldsymbol{\gamma}\cdot\boldsymbol{p}\ \left(\log\frac{\boldsymbol{p}^2}{\Lambda^2} - 4\log 2\right).$$

Insert an appropriate counterterm into the action (1) and express the resulting renormalized Fermi velocity $v_{\rm F}^{\rm ren}(\boldsymbol{p}^2)$ in terms of the bare Fermi velocity and the normalization scale μ.