Faculty of Physics, Lomonosov Moscow State University

Advanced Quantum Field Theory: Modern Applications in HEP, Astro & Cond-Mat
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Handout (Fall 2016 term) – FINAL VERSION

1. Relying upon the well-known theorem from quantum mechanics on simultaneous diagonalizability of *commuting Hermitian* operators, show that the (*non-Hermitian*) translation operator $\hat{T}_{\boldsymbol{d}} \equiv e^{\boldsymbol{d}\cdot\boldsymbol{\nabla}}$ has a complete orthonormalized set of eigenfunctions in $L_2(\mathbb{R}^3)$ that are also eigenfunctions of the Hamiltonian $\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\boldsymbol{x})$, $V(\boldsymbol{x}+\boldsymbol{d}) = V(\boldsymbol{x})$.

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., 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

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

   featuring the 'single-bond' and 'double-bond' hopping integrals u, v. Find the energy dispersion relation $\varepsilon(k)$ for this TB model (*Note: mind the unit cell first!*) and the effective mass for electrons ($\varepsilon > 0$).

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.

4. Find the ground-state energy of a helium atom using the Hartree–Fock–Roothaan equations based on (a) $1s$ orbitals, (b) orbitals with $n = 1, \ldots, n_{\max}$ for some reasonable $n_{\max}$; (c) using the post-Hartree–Fock configuration interaction scheme. Compare the energies and the RMS charge radii $\sqrt{\frac{1}{2}\int \rho(\boldsymbol{r})\mathrm{d}^3x}$ thus obtained ($\rho(\boldsymbol{x})$ is the total charge density of two electrons, in units of e).

5. Find the density profile $n(r)$ for an atom with the nucleus charge $-Ze$ using the Thomas–Fermi equation. Note: resort to spherically-symmetric solutions; find the form of the $r \to \infty$ and the $r \to 0$ asymptotics; estimate the unknown parameters in the asymptotic expressions numerically.

6. Find the leading coefficient g_0 in the exchange-correlation energy for the dilute homogeneous electron gas of density n,

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

7. 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

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

   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

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

8. Let us look at a hydrogen H_2 molecule from a Hubbard-model standpoint

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

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 four operators $\hat{\boldsymbol{S}}^2 = (\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2, \hat{S}_z = \hat{S}_{1z} + \hat{S}_{2z}, \hat{P}, \hat{N} = \sum_{i,\sigma} \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$ commute with each other and with $\hat{H}$, find the energies and wave functions for triplet $S = 1$ and singlet $S = 0$ states of the molecule. The spatial parity operator simply exchanges the two sites, $\hat{P}\hat{c}_{i\sigma}\hat{P} := \hat{c}_{3-i,\sigma}$. Compare your results with the TB ($U = 0$) case.

9. 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

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

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

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

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

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.

11. Consider *strained graphene* with the Hamiltonian

$$\hat{H} = -\sum_{\boldsymbol{x}\in A} \sum_{j=1,2,3} (t + \Delta t_j)\hat{b}^\dagger_\sigma(\boldsymbol{x} + \boldsymbol{\delta}_j)\hat{a}_\sigma(\boldsymbol{x}) + \text{h.c.}, \tag{1}$$

where $\boldsymbol{\delta}_{1,2,3}$ connect a site $\boldsymbol{x}$ of sublattice A with its nearest neighbours of sublattice B and $|\Delta t_j| \ll t$ (in general, $\Delta t_j \in \mathbb{C}$). In the leading order in $|\Delta t_j|/t$, find the shifted Fermi points (and justify that the Fermi surface is still degenerate, consisting of only two *points*). Introducing the wavefunction $\Psi_\sigma(\boldsymbol{x})$ containing the low-energy degrees of freedom, find the effective wave equation for it.

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

$$\Delta t_j \rightsquigarrow \Delta t_j(\boldsymbol{x}) = \kappa \left\{ e^{\mathrm{i}(\boldsymbol{Q}\cdot\boldsymbol{x} + \boldsymbol{k}_+\cdot\boldsymbol{\delta}_j)} + e^{\mathrm{i}(-\boldsymbol{Q}\cdot\boldsymbol{x} + \boldsymbol{k}_-\cdot\boldsymbol{\delta}_j)} \right\} \to 0, \qquad \boldsymbol{Q} \equiv \boldsymbol{k}_+ - \boldsymbol{k}_-,$$

in the above Hamiltonian (1). Find the modification of the effective Dirac equation resulting from such a perturbation (N.B.: it will mix the two Fermi points $\boldsymbol{k}_\pm$!).

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 $\sigma\mu_{\mathrm{B}}B$). 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

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