Lecture 2. Some Important (quasi-) 2D systems

A. Naturally Occurring

1. Graphene

A single sheet of C atoms – most "perfect" 2D system known to occur naturally. Although most experiments use graphene enscribed on some insulating substrate (e.g. SiC) it is perfectly possible to produce (att. μ -sized) free-standing (suspended) sheets^{*}.

Structure is honeycomb, (so 2 inequivalent sublattices), with C - Cseparation ~ 1.42Å. "Hardest" system known in nature. (breaking strength ~ 100 times that of steel) (^{\dagger} most expensive: \$100 M/cm² – by 2013, down to \sim \$60/ in²)



Chemistry: C. electronic str. $(ls^2)2s^22p^2$; of the 4 valence electrons, 3 form the 3 sp^2 bonds necessary to maintain the 120° bond configuration at each atom, leaving 1 per atom over. Thus, prima facie pure graphene should be metal with half-filled conduction band. Actually, more interestingly: band str. is peculiar, with a "Dirac point" exactly halfway up the band. Hence pure graphene is insulator, or more strictly a semimetal.



Easy to dope with either donor or acceptor impurities, i.e. provide extra electrons/holes. Mobility is enormous ($\sim 2.5 \times 10^5 \text{ cm}^2/V$ sec at RT.

From the point of view of basic physics, special interest of graphene is the nature of the electron states close to the D.P .:

 \widehat{H}_{eff} = const. $\sigma \cdot p$ (like Majorana neutrino) ($v_{\rm F}$ ~10⁶ m/sec)

⇒ many analogies with relativistic physics. Also v. interesting from applied point of view. Thus, enormous surge of interest (>60,000 papers since 2004).

2. Graphite

Basically the stuff of "lead" pencils: pure C sheets (i.e. graphene), sp²-bonded, honeycomb lattice, (hexagonal) lattice const. ~ 1.42Å, layer spacing (unintercalated) ~3.35Å. Interplane bonding is principally vdW, hence v. friable (although π -orbitals stick out of plane, they are antibonding, hence do not contribute much to interplane cohesion). Ratio of conductivities, $\sigma_1 / \sigma_{\parallel} \sim 3 \times 10^{-4}$. ($\sigma_{\parallel} \sim 10^4 - 10^5 \Omega^{-1} \text{ cm}^{-1}$ at RT); can be intercalated[‡] with e.g. alkalis or SbF₆; in latter case $\sigma_{\perp} / \sigma_{\parallel} \sim 10^{-6}$. Apart from intrinsic interest, useful substrate for e.g. He

[†] For comparison, μ of most semiconductors at RT – a few × 10³ (Kiltel, SSØ, p. 308).

^{*} See e.g. Meyer et al., Nature 446, 60 (2007).

[‡] Review of intercalated graphite: Dresselhaus et al., Adv. Phys. 30 (1980). Reprinted in Adv. Phys. 51, 1 (2002). Note σ of Cu at RT ~ 6×10⁵ Ω^{-1} cm⁻¹.

films. Sometimes superconducting but only at a fraction of a K. [but rises with intercalation (maximum app. ~ 0.55 K)]. [note: for graphite host, free carrier centration only $\sim 10^{-4}$ /atom at RT]

3. TM dichalcogenides*

These are of the formula MX_2 , where M is a group-V transition metal (usually Ta or Nb) and X is a chalcogen (usually S or Se): e.g. TaS_2 , $NbSe_2$.

(\uparrow : do not confuse with the TM trichalcogenides, such as *TaS*₃ and *NbSe*₃, which are essentially 1D systems). Composed of sheets of metal atoms sandwiched by the chalcogens.

Recall: electronic str. of *Ta* is $5d^36s^2$ and of *Nb* $4d^4$ 5s: so 4 of the 5 valence electrons form (double) ionic bonds with the 2 chalcogens (*S* is $3s^23p^4$, *Se* $4s^24p^4$, so 2 holes/atom), leaving 1 "free" e⁻ per formula unit \Rightarrow half-filled band. This e⁻ is essentially in a *d*-state and lives mainly in the plane of the metal atoms \Rightarrow expect system to be essentially 2D, with transport || plane easy and that along c-axis (\perp) difficult. In practice, $\sigma_{\perp}/\sigma_{\parallel} \sim 0.03$. (Absolute value of $\sigma_{\parallel} \sim 10^4 \Omega^{-1} \text{cm}^{-1}$ at RT, rising to $\sim 10^6 - 10^7 \Omega^{-1} \text{cm}^{-1}$ at low *T*, see FJ fig 13).

Calculated F.S. v flat along c-axis, as expected. However, also has parts which are v. flat in **plane**, so quite close to nesting (FJ fig 12). So not surprising that many such materials from CDW/s at low T. 2H polytype also superconducting at LT (≤ 1 K).

Easy to intercalate the TM chalcogenides, e.g. with flat organic molecules, and then superconducting T_c rises dramatically (to ~ 6K for TaS₂).

4. 2 D organics

Most Xtals made up of aromatic hydrocarbons likely to be strongly 2D. Polyacenes (benzene, naphthalene, anthracene, tetracene pentacene,...) insulating in natural state (HOMO-LUMO gap $\sim 2.5 - 4 \text{ eV}$).

However, most studied 2D organic Xtals are based on bis (ethylene-dithiol) – tetrathia fulvalene (BEDT-TTF \Rightarrow ET) and are of general formula

 $(ET)_2X$





when $X = (e.g.) I_3^-$, IBr_2^- , AuI_2^- , or more complex groups like $Cu - (NCS)_2$. Many types of str. (e.g. α , β , κ ...) even for same compound, but generally speaking Xtals tend to form layers of $(ET)_2$ separated by layers of X.

Review: Frickel & Jerome, J. Phys. C 12, 1441 (1979), section 3.4 ("FJ")

S

Band str. as calculated by TB method (or seen experimentally in dHvA, etc.) fairly close to cylindrical, with in-plane hopping matrix element $t_{\parallel} \sim 0.05$ eV.

Many of the 2D organics superconduct, with T_c up to ~14K. In view of small t_{\parallel} , this may be regarded as "high-temperature" superconductivity!

5. Cuprates[†]

The cuprates are a group of fairly strongly 2D materials whose main claim to fame is that many of them (~300 different compounds by now) show superconductivity at enormously high T (max ~ 160 K (Hg - 1223): dozens in range 110 – 120 K). Note that not all cuprates show HTS, and those that do generally show it only in a restricted range of doping (cf. below).

Composition: traditional chemical notation, e.g. $YBa_2Cu_3O_{7-\delta}$, not v. informative. More sensible to write generic formula for a cuprate in form

$$(CuO_2)_n A_{n-1}X$$
 $(n = 0, 1 ...)$

where A = alkaline earth, rare earth, Y, La..., X = (almost) anything (not necessarily stoichiometric), but frequently heavy-metal oxide.[‡]

 CuO_2 units occur in planes, with structure as shown. If more than 1 CuO_2 per (physical)§ unit cell, then they occur together (in "multilayers") special (intercalated) by the element A. The remainder of the formula, X, is the "charge reservoir" and lies between the "multilayers". In the literature one sometimes partitions the charge reservoir material into a "spacing" layer next to the CuO_2 planes, typically an oxide, and one or more "insulating" layers (which can actually be weakly metallic). E.g. in YBCO, where the reservoir is $BaCuO_{3-\delta}$, the spacing layers (near to the CuO planes) are BaO, and the (not very insulating!) "insulating"



layer is the $CuO_{1-\delta}$ chains. In some compounds, e.g. $La_2CuO_{4-\delta}$, the insulating layer is absent.

Electronic str.: It is often possible to construct, for a given choice of elements in the charge reservoir X, a stoichiometric compound s.t. the values balance, e.g. La_2CuO_4 or $YBa_2Cu_3O_6$ (note not O_7 !). When one balances the valences in this way, the Cu's (which started off in the $3d^{10}$ 4s configuration) are left in the Cu^{++} , $3d^9$ configuration, thus with 1 hole per CuO_2 unit in the d-shell. So band theory would predict that at least the single-layer compounds of this class, such as La_2CuO_4 , would be metals (since they have one odd electron per unit cell, hence a half-filled band). In fact, both La_2CuO_4 and $YBa_2Cu_3O_6$ are **insulators**, and all the evidence is that

^e cf. P.A. Lee, Reps. Prog. Phys. 71, 012501 (2008), p. 3.

[†] Ref.: Shaked et al., ANL "pocket book".

[‡] Thus, the compound usually called $YBa_2Cu_3O_{7-\delta}$ is in this notation $(CuO_2)_2 Y(BaCuO_3)$.

[§] The "crystallographic" unit cell is two physical unit cells.

they are Mott insulators (one localized e /unit cell) and moreover AF.

If now we deviate from exact stoichiometry, e.g. by setting $\delta \neq 0$ (YBCO) or by substituting say Sr for La (LSCO), the effect is to inject extra holes (or sometimes e^{-s}); those tend to sit in the planes, predominantly on the Cu sites, and hence are predominantly in one of the Cu 3d states: all the evidence is that they are specifically in the $d_x 2^{-y^2}$ state ($d_z 2^{-r^2}$ and d_{xy} , d_{xz} and d_{yz} states being already filled) and hybridize somewhat with the O $2p_x$ and $2p_y$ states.

Both because of the strongly anisotropic Xtal str., and because the "free" electrons are primarily in the $d_{x^2-y^2}$ state, the electronic properties of the cuprates are expected to be highly anisotropic, and indeed the experimental value of $\sigma_{\parallel}/\sigma_{\perp}$ ranges from ~ 30 (in optimally doped *YBCO*) to ~ 10⁵ (*Bi* 2212) (and even higher in some intercalated cuprates)*. Typically $\sigma_{\parallel} \sim 10^3$ S/cm at *RT* (and "optimal" doping) (~10⁻³ that of *Cu*); interestingly, this correlates to a R_0 per square of *CuO2* plane which is of the order of the "quantum unit of resistence" h/e^2 (lecture 5).

[In addition to superconductivity, weak localization may be observable in cuprates.]

6. Strontium ruthenate[†] (Sr_2RuO_4)

Original motivation for study: similarity in both structure and chemistry to cuprates. Structure is layered, with RuO_2 planes separated by SrO_2 spacers (so similar to e.g. La_2CuO_4), similar plane spacing (~ 6Å).

Chemistry: Cu(Z=29) is $[Ar] + 3d^{10}4s^1 \rightarrow 3d^9$

Ru(Z = 44) is $[Kr] + 4d^{7}5s^{1} \rightarrow 4d^{4}$

In normal state, $\sigma_{\perp}/\sigma_{\parallel} \sim 10^{-3}$ (similar to cuprates), (but *T*-dependence in each case nothing like cuprates). Residual resistance ~ 1 $\mu \Omega$ cm (comparable to *Cu* at *RT*).

Becomes superconducting at $T_c \sim 1 \text{K}$ (cuprates: ~ 100 K!)

Most interesting feature: strong evidence that Cooper pairs form in **spin triplet** state, and moderately strong evidence (inc. Kidwingira et al.) that they form in the so-called (p + ip) orbital states. Hence of great interest in context of TQC.

(like 3*He-A*, but 2-dimensional so no nodes in gap)

7. Films of liquid He But 2-dimensional so no nodes in gap

Neither ³*He* nor ⁴*He* crystallizes under own vapor pressure \rightarrow can (inter alia) form liquid film on certain kinds of substrate (e.g. graphite, metallic, Cs). General belief is that first 2 layers are "solid", not "liquid" (but conceptual problem regarding the meaning of solid/liquid in this kind of situation). On some substrates however evidence for superfluidity of ⁴He (hence, a fortiori

^{*} All the evidence is that the electronic transport in the $C(\perp)$ direction is by incoherent hopping, so that the concept of a BS is inapplicable.

[†] Comprehensive review: Mackenzie & Maeno, RMP 75, 1 (2003).

"liquidity") down to a fraction of a monolayer.

A related 2D system is **electrons** on the **surface** of liquid *He* (typically v. low density, $\sim 10^{-9}$ cm⁻²)

8. Monolayers (of rare gases tc)*

Although in bulk all elements other than *He* (including the other rare gases, *Ar*, *Ne*, *Xe*...) form solids, it is often possible to put down monolayer or sub-monolayer amounts on some appropriate surface (e.g. exfoliated graphite) and measure properties such as the specific heat or NMR. Many of these systems show interesting phase transitions between solid/liquid or commensurate/incommensurate phases.

9. Ferropnictides

Superconductivity in this group of materials was discovered in January 2008: it shows the highest T_c (~ 55K, but see also below) of any non-cuprate material[†]. All compounds in this class contain a transition metal (usually Fe)[‡] and a pnictide element (same column of periodic table as N), usually As, or a chalcogenide (Se or Te). By now four classes of ferropnictides have been discovered, denoted respectively by "1111", "122", "111" and "11." The 1111 class is derived from a parent compound with the formula

(RE)(TM)(PN)O RE \equiv rare earth, TM \equiv transition metal, PN \equiv pnictide, O \equiv oxygen

A typical example is

LaFeAsO ("iron oxypnictides")

This class is not superconducting in the parent state, but becomes so when some of the O is replaced by F: LaFeAsO_{1-x}F_x and then can have T_c up to ~ 55K (SmFeAsO_{1-x}F_x, $x \approx 0.15$). (also pure O deficiency)

The second class, "122" has the formula $(AE)(TM)_2(PN)_2$ (AE \equiv alkaline earth): example is BaFe₂As₂. This class is (sometimes) superconducting in the parent state, but with a low T_c (a few K); T_c can be raised to ~ 38K by partial substitution of the AE by an alkali, e.g. $(Ba_{1-x}K_x)Fe_2As_2$. A third class, "111" has the formula A(TM)(PN) (A \equiv alkali), e.g. LiFeAs. In this case, superconducting transition temperatures up to ~ 20K are reached already in the pure stoichiometric material without chemical doping. Finally, there is a class "11" with the simple formula (TM)C (C \equiv chalcogenide), e.g. Fe Se.; note that this class contains no As, although the structure of the Fe Se (etc.) planes seems to be very similar to that of the Fe As planes in the other ferropnictides (on which see below).

In the first year or so of the subject, most experimental work was done on the "1111" compounds; however, following the discovery that unlike these the 122's could be prepared as large single crystals, attention has tended to shift to them. Less work has been done on the 111 and 11 classes, in the latter case partly because the behavior seems extremely sensitive to small variations in doping and disorder. However, recently FeSe monlayers have attracted considerable interest (see below).

^{*} Cf. Thouless op. cit.

[†] Except for the very recently discovered HS System.

¹ LaNiPo is superconducting but only at 4 – 5K.

Structure and chemistry

The 1111 compounds crystallize in the so-called ZrCuSiAs structure; within each unit cell we have a "LaO layer" (roughly, two La planes sandwiching an O plane) and a "FeAs layer" (2 As planes sandwiching an Fe plane). In the tetragonal phase (see below) the ab-plane lattice constant is ~ 4 Å, the c-axis l.c. ~ 9Å (cf. the cuprates). See Figs. 1 and 2 The Fe-Fe spacing is ~ 2.85Å. In the parent compound (e.g. LaFeAsO) the ionization state³ is believed to be $(La^{3+}O^{2-})^+(Fe^{2+}As^{3-})^-$, i.e. the LaO layer is (doubly) closed-shell, the As is (roughly) closed-shell and the Fe is $3d^6$. There is believed to be some hybridization between the 5 Fe 3d states and the As 4p's. When F (Z = 9) is substituted for O (Z = 8), the extra electron is believed to migrate to the FeAs layer, giving (at $x \sim 0.1$) a carrier density (above the parent compound) of ~ 10^{21} cm⁻³. This number, and also the fact that the "charge reservoir" (in this case the LaO layer) is well separated from the metallic (FeAs) layer, is similar to (some of) the cuprates; however, note that the 1111 series is *electron*-doped.⁴

In the 122 compounds (e.g. $CaFe_2As_2$), the unit cell $(a = 3.9\text{\AA}, c = 11.7\text{\AA})$ contains two similar layers, each of them with two planes sandwiching an Fe plane, separated by an alkaline-earth plane. (Again, the charge reservoir ($Ca \rightarrow K$) layer is relatively distant from the Fe atoms.) Note that substitution of an AE by an alkali (e.g. $Ca_{1-x}K_x$) gives hole doping, as in the cuprates and again, for $x \sim 0.1$ the (extra) carrier density is $\sim 10^{21} \text{cm}^{-3}$.

Note that in the 1111 compounds many RE's are possible (La, Sm, Ce, Nd, Pr, Gd) (though T_c may be only ~ a few K, e.g. for Gd); in the 122's Ba, Ca, Sr work.

(note influence of development of MBE on 2D physics)

1. Semiconductor interfaces

The great advantage of semiconductors over metals is that because of the low density and hence relatively poor screening properties, it is easy to influence the carrier density close to a surface by applying modest potentials (~ a few V) and thereby bending the bands over an energy quite comparable to the intrinsic band gap. (Nb: band gap of $Si = 1.14 \ eV$, binding en of B acceptor = 0.045 eV)

Si MOSFETs

This is probably the conceptually simplest case.

A positive potential applied to the metal bends the bands, as shown. The ptype Si contains acceptor impurities (e.g. B) which



⁹Recall: Fe: 3d⁶4s², As: 4s²4p³, La: 5d6s², Sm: 4f⁶6s²

⁴But hole-doping is also sometimes possible, e.g. La \rightarrow La_{1-x}Sr_x, $T_c = 25$ K (cf. cuprates)

are ionized, so there is a nonzero concentration of holes in the bulk, but close enough to the surface, the potential for holes drives them away, giving a "depletion layer" which is insulating. Meanwhile, if the applied potential exceeds

 $E_b - \mu$, there will be a region (shaded) close to the surface where the electron energy is $< \mu$, thus it will be advantageous for electrons from the metal to migrate there. ("inversion layer")

The width of the inversion layer is typically ~25 Å, and the electrons have to a first approximation their bulk-*Si* values of m* (~0.2 m) and also \in (~12). Hence the energy of the first excited transverse state is ~200K. Mobilities can be high, ~ 10⁶ cm²/V sec, corresponding to a mfp ~ 5 μ .

GaAs-GaAlAs (Al_xGa_{1-x}As) heterstructures.

Note that although "quantum wells" are often mentioned in this context, all that is really needed is an interface between two semiconductors with appreciably different band gaps. We dope the *AlGaAs* with donor impurities, which became ionized and thus generate an (approximately quadratic) potential (div $E = \rho/\epsilon_0 \Rightarrow E \sim \rho(x - x_0) \Rightarrow \phi$ $\sim \rho(x - x_0)^2$). The donated electrons migrate to the point of lowest potential, on the *GaAs* side of the interface. The confinement region typically has width ~ 200 Å, and the effective



mass of an e^- in bulk *GaAs* is *~0.07 m (and \in ~ 11), so the en. of the first excited state is ~ 10K. Densities (controllable by gate voltage) are typically ~ $10^{10} - 10^{12} e^{-1}$ cm²: note that this means that in a \perp 'r magnetic field of a few *T*, the filling factor is ~1.

An advantage of this geometry is that the electrons filling the surface states are spatially separated from their donors. As a result mobilities can be v. high indeed ($-3 \times 10^7 \text{ cm}^2/V$ sec in recent experiments), higher even than attained in the best Si = MOSFETs. Another advantage of this system vis-à-vis. Si is that in the latter than are 2 different "valleys", with awkward geometrical! props, while in GaAs there is only one valley centered on the Γ point of the FBZ. For these reasons, GaAs/AlGaAs heterostructures have in recent years become the system of choice for sophisticated QHE experiments.

Engineered systems, cont.

Trapped ultracold atomic gases

Ultracold atoms may be trapped by a spatially varying magnetic field and/or by counterpropagating laser beams. In the case of magnetic trapping the relevant potential is just $-\mu \cdot B(r)$ where μ is the atomic magnetic moment. Since it is impossible to produce a maximum of the (time-independent) magnetic field in free space (Earnshaw's theorem) but perfectly possible to produce a minimum, one usually tries to trap atoms in the hyperfine states in which μ

is **oppositely** oriented to the field (the "low-field seekers"); contrary to what one might perhaps think, these hyperfine states are often stable over timescales ~ minutes (comparable to the decay time of the gas). In the case of optical trapping, the basic principle is that if the detuning $\Delta \equiv \omega_{\text{las}} - \omega_{\text{tr}}$ of the laser field from the relevant atomic transition is \gg the spontaneous linewidth Γ of the transition, then after averaging over timescales $\gg \omega_{\text{laser}}^{-1}$ one gets an effective potential which is proportional to I_0/Δ where I_0 is the laser intensity at the point in question. Note (a) the potential is repulsive (attractive) for blue-shifted (red-shifted) laser frequencies (b) the intensity is proportional to the square of the [(optically averaged)] **total** electric field **E**, thus by using counterpropagating beams one can get a strong spatial dependence of the trapping potential. If the laser wavelength is λ_L and the two beams are propagating at relative angle θ , then one gets a periodic potential with "periodicity" $\lambda_L / (2 \sin \theta)$. This potential has a depth (height) V_0 which is normally expressed in terms of the "recoil" energy $E_R \equiv \hbar^2 k_L^2 / 2M$ where $k_L \equiv 2\pi / \lambda_L$ and Mis the mass of the atom in question: a typical value of E_R is ~ 5kHz (200 *nK*), and typical values of V_0/E_R range from 0 to~40. The potential is sinusoidal, and the frequency of small oscillations around the minimum is $2\sqrt{V_0E_R} / \hbar$.

In order to get an effectively 2D system, one combines magnetic trapping in all 3 dimensions with laser trapping in one direction (\perp 'r to the desired 2D planes). Thus, in the experiment of Hadzibabic et al.^{*}, a cloud of ⁸⁷Rb atoms was subjected to a total potential

where

$$V(r) = V_{\text{mag}}(r) + V_{\text{laser}}(r)$$

$$W_{\rm mag}(r) \cong \frac{1}{2} M \left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right)$$

$$V_{\text{laser}}(r) \cong V_0 \exp\left(-2x / W_x^2\right) \sin^2 k \left(z - z_0\right)$$

where W_x is the laser "waist" along the x – direction and z_0 is the offset of the laser potential (which does not necessarily coincide with the minimum of the magnetic potential). The parameters of the experiment were

 $V_0 / \hbar = 50 kHz$, $\omega_x / 2\pi = 11 Hz$, $\omega_y = 130 Hz$, $\omega_2 = 3.6 kHz$, lattice period $\pi/k = 3\mu$, (so $\omega_z \gg \omega_x, \omega_y$ i.e. magnetic z-trapping is much stronger than the in-plane trapping). (In the actual experiment, they often set a **maximum** of the potential at z_0 , so as to obtain 2 degenerate minima). Bearing in mind that 20 kHz corresponds to 1 μK , we see that at 80 nK (a typical temperature in the experiment) the second harmonic oscillation in the z-direction is only very weakly thermally excited, so indeed the system can be regarded as "2D".

^{*} Nature 441, 118 (2006) c.f. also NJP 10, 045506 (2008)

A major difference between optically trapped atomic gases and solid-state systems is that in the former case the "system" can be rapidly taken apart by turning off the potentials: this is extremely useful in diagnosing its behavior, e.g. by looking for interference effects.

Diagnostics of (quasi-) 2D systems

The question of experimental methods available for examination of the structure and dynamics of (quasi-) 2D systems is liable to depend heavily on whether we are dealing with a single system (e.g. graphene, *He* films, QHE systems) or with a macroscopically large number of similar systems embedded in a 3D matrix (e.g. organics, cuprates). In the latter case most of the standard techniques of condensed matter physics are available: e.g. X-ray/neutron scattering can be used to probe the structure, and at least if we can reliably subtract the contribution of the matrix, thermodynamic quantities such as the specific heat c_v and spin susceptibility χ can be measured.

For genuinely isolated single 2D systems most of these methods are impractical, simply because the number of atoms/electrons involved is too small. However, this difficulty should not be overestimated: remarkably, it is possible to examine the structure of even a single suspended graphene sheet by TEM^{*}, and which conventional NMR in (say) QHE systems is impossible because of the weakness of the signal, resistively detected NMR has been used[†] to measure the spin susceptibility of some the more robust QH states.

The most commonly used diagnostic for (quasi-) 2D systems is the transport properties. In the case of a film / monolayer on a substrate, the thermal conductivity is likely to be shorted out by the substrate, but for free-standing films it should be measureable. Even in the case of a substrate, provided it is insulating, the electrical conductivity of the 2D system is relatively easy to measure, and so is the Hall conductivity. In the case of the QHE, in fact, until recently these have been just about the only things that can be measured. In principle, optical absorption and photoconductivity should be measurable.

^{*} J.C. Meyer et al., Nature **446**, 60 (2007).

[†] E.g. R. Côté et al, PRB **93**, 075305 (2016)