1 Time reversal

1.1 Without spin

Time-dependent Schrödinger equation:

$$i\hbar\partial_t\psi\left(\mathbf{r},t\right)=\left[-\frac{\hbar^2}{2m}\Delta+V\left(\mathbf{r}\right)\right]\psi\left(\mathbf{r},t\right) \tag{1}$$

'Local' time-reversal transformation, T:

$$t_1<t_2<\ldots<t_n\Rightarrow Tt_1>Tt_2>\ldots>Tt_n \tag{2}$$
$$Tt_i-Tt_j=-\left(t_i-t_j\right) \tag{3}$$
$$T=T^{-1} \tag{4}$$

$$\Downarrow$$

$$\frac{df\left(T\circ t\right)}{dt}=\lim_{dt\to0}\frac{f\left(Tt+Tdt\right)-f\left(Tt\right)}{dt}=\lim_{dt\to0}\frac{f\left(Tt-dt\right)-f\left(Tt\right)}{dt}=-\left.\frac{df\left(t\right)}{dt}\right|_{Tt} \tag{5}$$

For simplicity, we will denote $\left.\frac{df(t)}{dt}\right|_{Tt}$ by $\frac{df(Tt)}{dt}$, which should not be confused with $\frac{df(T\circ t)}{dt}$!
The time-reversed Schrödinger equation then reads as

$$-i\hbar\partial_t\psi'\left(\mathbf{r},Tt\right)=\left[-\frac{\hbar^2}{2m}\Delta+V\left(\mathbf{r}\right)\right]\psi'\left(\mathbf{r},Tt\right)\ . \tag{6}$$

On the other hand,

$$-i\hbar\partial_t\psi^*\left(\mathbf{r},t\right)=\left[-\frac{\hbar^2}{2m}\Delta+V\left(\mathbf{r}\right)\right]\psi^*\left(\mathbf{r},t\right) \tag{7}$$

$$\Downarrow$$

$$\psi'\left(\mathbf{r},Tt\right)=C\,\psi\left(\mathbf{r},t\right)\doteq\psi^*\left(\mathbf{r},t\right)\ . \tag{8}$$

Properties of the operator C:

$$C^2=1\,,C^{-1}=C\,, \tag{9}$$

C is anti-hermitian,

$$\langle\psi|C\varphi\rangle=\langle\varphi|C\psi\rangle=\langle C\psi|\varphi\rangle^* \tag{10}$$

and anti-linear,

$$C\left(c_1\varphi_1+c_2\varphi_2\right)=c_1^*C\varphi_1+c_2^*C\varphi_2\ . \tag{11}$$

However, the C preserves the norm of the wavefunctions,

$$\langle C\psi|C\psi\rangle=\langle\psi|\psi\rangle\ . \tag{12}$$

Relationship to other operators:

$$C\left(\mathbf{r}\psi\right)=\mathbf{r}\left(C\psi\right)\Longrightarrow C\mathbf{r}=\mathbf{r}C\Longrightarrow\left[\mathbf{r},C\right]=0 \tag{13}$$

Notation:

$$\mathbf{r}^* \mathrel{\hat{=}} C\mathbf{r}C = \mathbf{r}\,.$$

Furthermore,

$$C\left(\mathbf{p}\psi\right) = C\left(\frac{\hbar}{i}\nabla\psi\right) = -\frac{\hbar}{i}\nabla C\psi = -\mathbf{p}\left(C\psi\right) \Longrightarrow C\mathbf{p} = -\mathbf{p}C \Longrightarrow \mathbf{p}^* = -\mathbf{p} \tag{14}$$

$$C\mathbf{L} = C\left(\mathbf{r}\times\mathbf{p}\right) = \mathbf{r}\times C\mathbf{p} = -\left(\mathbf{r}\times\mathbf{p}\right)C = -\mathbf{L}C \Longrightarrow \mathbf{L}^* = -\mathbf{L}\,. \tag{15}$$

1.2 With spin

Pauli-Schrödinger Hamilton operator

$$H = \frac{\mathbf{p}^2}{2m} + V\left(\mathbf{r}\right) + \frac{\mu_B}{\hbar}\left(\mathbf{L}+2\mathbf{S}\right)\mathbf{B} \tag{16}$$

Pauli-Schrödinger equation

$$i\hbar\partial_t\psi\left(\mathbf{r},t\right) = \left[-\frac{\hbar^2}{2m}\Delta + V\left(\mathbf{r}\right) + \frac{\mu_B}{\hbar}\left(\mathbf{L}+2\mathbf{S}\right)\mathbf{B}\right]\psi\left(\mathbf{r},t\right) \tag{17}$$

Time-reversed magnetic field: $\mathbf{B}' = -\mathbf{B}$! The time-reversed Pauli-Schrödinger equation then takes the form,

$$-i\hbar\partial_t\psi'\left(\mathbf{r},Tt\right) = \left[-\frac{\hbar^2}{2m}\Delta + V\left(\mathbf{r}\right) + \frac{\mu_B}{\hbar}\left(\mathbf{L}+2\mathbf{S}\right)\mathbf{B}'\right]\psi'\left(\mathbf{r},Tt\right) \tag{18}$$

$$= \left[-\frac{\hbar^2}{2m}\Delta + V\left(\mathbf{r}\right) - \frac{\mu_B}{\hbar}\left(\mathbf{L}+2\mathbf{S}\right)\mathbf{B}\right]\psi'\left(\mathbf{r},Tt\right)\ . \tag{19}$$

On the other hand,

$$-i\hbar\partial_t\psi^*\left(\mathbf{r},t\right) = \left[-\frac{\hbar^2}{2m}\Delta + V\left(\mathbf{r}\right) + \frac{\mu_B}{\hbar}\left(\mathbf{L}^*+2\mathbf{S}^*\right)\mathbf{B}\right]\psi^*\left(\mathbf{r},t\right) \tag{20}$$

$$= \left[-\frac{\hbar^2}{2m}\Delta + V\left(\mathbf{r}\right) - \frac{\mu_B}{\hbar}\left(\mathbf{L}-2\mathbf{S}^*\right)\mathbf{B}\right]\psi^*\left(\mathbf{r},t\right) \tag{21}$$

It is then tempting to suppose that $\exists\,\mathsf{M}\in\mathcal{L}\left(\mathbb{C}^2\right)$ such that

$$\psi'\left(\mathbf{r},Tt\right) = \mathsf{M}C\,\psi\left(\mathbf{r},t\right) = \mathsf{M}\,\psi^*\left(\mathbf{r},t\right)\ . \tag{22}$$

Since M acts only in spin space, it commutes with $\mathbf{r}$, $\mathbf{p}$ and $\mathbf{L}$. Thus,

$$-i\hbar\,\mathsf{M}\partial_t\psi^*\left(\mathbf{r},t\right) = \left[-\frac{\hbar^2}{2m}\Delta + V\left(\mathbf{r}\right) - \frac{\mu_B}{\hbar}\left(\mathbf{L}-2\mathbf{S}\right)\mathbf{B}\right]\mathsf{M}\psi^*\left(\mathbf{r},t\right) \tag{23}$$

$$\Downarrow$$

$$-i\hbar\partial_t\psi^*\left(\mathbf{r},t\right) = \left[-\frac{\hbar^2}{2m}\Delta + V\left(\mathbf{r}\right) - \frac{\mu_B}{\hbar}\left(\mathbf{L}+2\mathsf{M}^{-1}\mathbf{S}\mathsf{M}\right)\mathbf{B}\right]\psi^*\left(\mathbf{r},t\right)\ . \tag{24}$$

This equation is obviously satisfied if

$$\mathsf{M}^{-1}\mathbf{S}\mathsf{M}= -\mathbf{S}^{*} = -C\,\mathbf{S}\,C \Longrightarrow \mathbf{S}\,\mathsf{M}C = -\mathsf{M}C\,\mathbf{S}\,. \tag{25}$$

Let's define the time-reversal operator as $T \mathrel{\hat{=}} \mathsf{M}C$,

$$T\mathbf{S} = -\mathbf{S}T\ . \tag{26}$$

It is easy to prove that

$$T = e^{i\theta}\sigma_y\,C \tag{27}$$

for any $\theta \in \mathbb{R}$ is a general solution of Eq. (26). In most text-books $\theta = \frac{\pi}{2} \rightarrow T = i\sigma_y\,C$ is chosen, but in these notes we take $\theta = 0 \rightarrow T = \sigma_y\,C$.

Proof:

$$\sigma_x^* = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x \quad \sigma_y^* = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} = -\sigma_y \quad \sigma_z^* = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z \tag{28}$$

$$\Downarrow$$

$$T^{-1}\sigma_x T = (-\sigma_y C)\,\sigma_x\,(\sigma_y C) = \sigma_y\sigma_x\sigma_y = -\sigma_x \tag{29}$$

$$T^{-1}\sigma_y T = (-\sigma_y C)\,\sigma_y\,(\sigma_y C) = -\sigma_y \tag{30}$$

$$T^{-1}\sigma_z T = (-\sigma_y C)\,\sigma_z\,(\sigma_y C) = \sigma_y\sigma_z\sigma_y = -\sigma_z\,. \tag{31}$$

Properties:

$$T^{-1} = C\sigma_y = \sigma_y^* C = -\sigma_y C = -T \tag{32}$$

$$\Downarrow \tag{33}$$

$$T^2 = -1\,. \tag{34}$$

From the relationship,

$$\begin{aligned}\langle\psi|T\varphi\rangle = \langle\psi|\sigma_y C\varphi\rangle = \langle\sigma_y\psi|C\varphi\rangle = \left(\sigma_y^{rs}\right)^* \langle\psi_s|C\varphi_r\rangle = \left\langle\varphi_r|C\sigma_y^{rs}\psi_s\right\rangle \\ = \langle\varphi|C\sigma_y\psi\rangle = -\langle\varphi|T\psi\rangle = -\langle T\psi|\varphi\rangle^*\ ,\end{aligned} \tag{35}$$

it follows that

$$\langle\psi|T\psi\rangle = -\langle\psi|T\psi\rangle = 0\ , \tag{36}$$

i.e. ψ and $T\psi$ are orthogonal. Note also that T is antiunitary,

$$\langle\psi|\varphi\rangle = \left\langle\psi|TT^{-1}\varphi\right\rangle = -\left\langle T\psi|T^{-1}\varphi\right\rangle^* = \langle T\psi|T\varphi\rangle^* = \langle T\varphi|T\psi\rangle$$

and norm-conserving,

$$\langle T\psi|T\psi\rangle = -\left\langle\psi|T^2\psi\right\rangle = \langle\psi|\psi\rangle\ . \tag{37}$$

The momentum operators and angular momentum operators change sign upon time reversal:

$$T^{-1}\mathbf{p}T = C\sigma_y\mathbf{p}\sigma_y C = C\mathbf{p}C = -\mathbf{p} \Longrightarrow \mathbf{p}T = -\mathbf{p}T \tag{38}$$

$$T^{-1}\mathbf{L}T = C\sigma_y\mathbf{L}\sigma_y C = C\mathbf{L}C = -\mathbf{L} \Longrightarrow \mathbf{L}T = -\mathbf{L}T\,, \tag{39}$$

thus the Hamilton operator with magnetic field $\mathbf{B}$ transforms to that with $-\mathbf{B}$,

$$TH(\mathbf{B}) = T\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) + \frac{\mu_B}{\hbar}(\mathbf{L}+2\mathbf{S})\mathbf{B}\right) = \left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) - \frac{\mu_B}{\hbar}(\mathbf{L}+2\mathbf{S})\mathbf{B}\right)T = H(-\mathbf{B})T\,, \tag{40}$$

or

$$T^{-1}H(\mathbf{B})T = H(-\mathbf{B}) \ . \tag{41}$$

This is the manifestation that time reversal changes the sign of the magnetic field. This is valid even in the presence of spin-orbit coupling,

$$H_{SO} = \frac{\hbar}{4m^2c^2}(\nabla V \times \mathbf{p})\boldsymbol{\sigma}\,, \tag{42}$$

since

$$\begin{aligned} T^{-1}(\nabla V \times \mathbf{p})\boldsymbol{\sigma}T &= \left(T^{-1}(\nabla V \times \mathbf{p})T\right)\left(T^{-1}\boldsymbol{\sigma}T\right) \\ &= (\nabla V \times (-\mathbf{p}))(-\boldsymbol{\sigma}) = (\nabla V \times \mathbf{p})\boldsymbol{\sigma}\ , \end{aligned} \tag{43}$$

i.e. H_{SO} also commutes with T.

Corollary 1: The Hamilton operator of a system is time-reversal invariant only in the absence of external magnetic field (or spontaneous spin-polarization (exchange splitting) that couples only to the spin of electrons, $H_{sp} = \frac{2\mu_B}{\hbar}\mathbf{S}\mathbf{B}_{ex}$).

Corollary 2: If $\psi_n(\mathbf{B})$ is an eigenstate of $H(\mathbf{B})$,

$$H(\mathbf{B})\psi_n(\mathbf{B}) = \varepsilon_n(\mathbf{B})\psi_n(\mathbf{B}) \tag{44}$$

then $T^{-1}\psi_n(\mathbf{B})$ is the eigenstate of $H(-\mathbf{B})$ with the same energy,

$$T^{-1}H(\mathbf{B})TT^{-1}\psi_n(\mathbf{B}) = H(-\mathbf{B})T^{-1}\psi_n(\mathbf{B}) = \varepsilon_n(\mathbf{B})T^{-1}\psi_n(\mathbf{B}) \ . \tag{45}$$

This implies that the spectra of $H(\mathbf{B})$ and $H(-\mathbf{B})$ are identical, i.e. the energy of a system does not change if the magnetic field is reversed.

1.3 Kramers degeneracy

Let us consider an eigenfunction, $\psi(\mathbf{r}_1 s_1, \ldots, \mathbf{r}_N s_N)$ of the N-electron Hamiltonian,

$$H\psi = \varepsilon\psi \tag{46}$$

being *invariant upon time reversal*,

$$T^{-1}HT = H \ . \tag{47}$$

The time-reversed wavefunction, $T\psi$, is then also eigenfunction of H with the same eigenvalue,

$$T^{-1}HT\psi = E\psi \Longrightarrow H(T\psi) = \varepsilon(T\psi) \ . \tag{48}$$

The time reversal operator T of the many-electron system should satisfy

$$T\mathbf{S}^{(k)} = -\mathbf{S}^{(k)}T\ , \tag{49}$$

for any $k = 1, \ldots, N$, where $\mathbf{S}^{(k)} = \frac{\hbar}{2}\boldsymbol{\sigma}^{(k)}$ is the spin operator of electron k. It is prove to see that T can be represented as

$$T = \sigma_y^{(1)} \ldots \sigma_y^{(N)} C\,. \tag{50}$$

since $\boldsymbol{\sigma}^{(k)}$ and $\boldsymbol{\sigma}^{(k')}$ commute for $k \neq k'$. The we can derive,

$$T = \sigma_y^{(1)} \ldots \sigma_y^{(N)} C = (-1)^N C\sigma_y^{(1)} \ldots \sigma_y^{(N)} = (-1)^N T^{-1} \implies T^2 = (-1)^N \ , \tag{51}$$

consequently,

$$T^{-1} = (-1)^N T\ .$$

This then implies,

$$\begin{aligned} \langle \psi | T\psi \rangle &= \left\langle \psi | \sigma_y^{(1)} \ldots \sigma_y^{(N)} C\psi \right\rangle = \left\langle \sigma_y^{(1)} \ldots \sigma_y^{(N)} \psi | C\,\psi \right\rangle \underset{\text{Eq. (10)}}{=} \left\langle \psi | C\sigma_y^{(1)} \ldots \sigma_y^{(N)}\,\psi \right\rangle \\ &= (-1)^N \left\langle \psi | \sigma_y^{1} \ldots \sigma_y^{N} C\,\psi \right\rangle = (-1)^N \langle \psi | T\psi \rangle\ . \end{aligned} \tag{52}$$

Corollary: For *odd number of electrons* ψ and $T\psi$ are orthogonal, therefore, the eigenstates of the system are at least twofold degenerate.

1.4 Kramers degeneracy of Bloch-states

We consider the Hamiltonian derived from the Dirac equation up to first order of $1/c^2$:

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) - \frac{\mathbf{p}^4}{8m^3c^2} + \frac{\hbar^2}{8m^2c^2}\Delta V(\mathbf{r}) + \frac{\hbar}{4m^2c^2}\left(\nabla V(\mathbf{r}) \times \mathbf{p}\right)\sigma\,, \tag{53}$$

where the third, fourth and fifth terms represent the relativistic kinetic energy correction, the Darwin term and the spin-orbit coupling, respectively. This one-electron Hamiltonian is invariant w.r.t. time-reversal,

$$T^{-1}HT = H\ . \tag{54}$$

In the previous section we learned that the eigenstates are at least two-fold degenerate:

$$H\psi = \varepsilon\psi \tag{55}$$

$$H(T\psi) = \varepsilon(T\psi) \tag{56}$$

and $T\psi$ is orthogonal to ψ.

A Bloch-state eigenfunction is defined as

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}}u_{\mathbf{k}}(\mathbf{r}) \tag{57}$$

$$H_{\mathbf{k}}u_{\mathbf{k}} = \varepsilon_{\mathbf{k}}u_{\mathbf{k}}\,,\ u_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{\mathbf{k}}(\mathbf{r})\ , \tag{58}$$

where the $\mathbf{k}$-dependent Hamiltonian for a non-spinpolarized periodic solid is,

$$H_{\mathbf{k}} = \frac{(\mathbf{p} + \hbar\mathbf{k})^2}{2m} + V(\mathbf{r}) - \frac{(\mathbf{p} + \hbar\mathbf{k})^4}{8m^3c^2} + \frac{\hbar^2}{8m^2c^2}\Delta V(\mathbf{r}) + \frac{\hbar}{4m^2c^2}\left(\nabla V(\mathbf{r}) \times (\mathbf{p} + \hbar\mathbf{k})\right)\sigma\,. \tag{59}$$

It is straightforward to show that

$$T^{-1}H_{\mathbf{k}}T = H_{-\mathbf{k}}\,, \tag{60}$$

therefore,

$$T^{-1}H_{\mathbf{k}}u_{\mathbf{k}} = \varepsilon_{\mathbf{k}}T^{-1}u_{\mathbf{k}} \tag{61}$$

$$\Downarrow$$

$$H_{-\mathbf{k}}\left(T^{-1}u_{\mathbf{k}}\right) = \varepsilon_{\mathbf{k}}\left(T^{-1}u_{\mathbf{k}}\right) \tag{62}$$

$$\Downarrow$$

$$\varepsilon_{-\mathbf{k}} = \varepsilon_{\mathbf{k}}\,, \tag{63}$$

and the two degenerate wavefunctions are:

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}}\begin{pmatrix} u_{\mathbf{k}+}(\mathbf{r}) \\ u_{\mathbf{k}-}(\mathbf{r}) \end{pmatrix} \quad \text{and} \quad \psi^{(1)}_{-\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{kr}}\begin{pmatrix} iu^{*}_{\mathbf{k}-}(\mathbf{r}) \\ -iu^{*}_{\mathbf{k}+}(\mathbf{r}) \end{pmatrix}\,. \tag{64}$$

1.5 Space inversion

Let's consider the case when also *space inversion* (i) applies:

$$V(i\,\mathbf{r}) = V(-\mathbf{r}) = V(\mathbf{r}) \tag{65}$$

$$\nabla V(i\,\mathbf{r}) = -\nabla V(\mathbf{r}) \tag{66}$$

$$\Delta V(i\,\mathbf{r}) = \Delta V(\mathbf{r}) \tag{67}$$

$$i\,(\mathbf{p}\,f(\mathbf{r})) = -\mathbf{p}\,f(-\mathbf{r}) \tag{68}$$

$$\Downarrow$$

$$i\,(H_{\mathbf{k}}(\mathbf{r})\,u_{\mathbf{k}}(\mathbf{r})) = H_{-\mathbf{k}}(\mathbf{r})\,u_{\mathbf{k}}(-\mathbf{r}) \tag{69}$$

$$\Downarrow$$

$$H_{-\mathbf{k}}(\mathbf{r})\,u_{\mathbf{k}}(-\mathbf{r}) = \varepsilon_{\mathbf{k}}u_{\mathbf{k}}(-\mathbf{r})\ . \tag{70}$$

Similar to time-reversal this implies that

$$\varepsilon_{-\mathbf{k}} = \varepsilon_{\mathbf{k}} \tag{71}$$

and also

$$u_{-\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(-\mathbf{r})\ .$$

The corresponding Bloch-eigenfunction for $-\mathbf{k}$ is given by,

$$\psi^{(2)}_{-\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{kr}}\begin{pmatrix} u_{\mathbf{k}+}(-\mathbf{r}) \\ u_{\mathbf{k}-}(-\mathbf{r}) \end{pmatrix}\,. \tag{72}$$

In case of both time-reversal and inversion symmetry, the two eigenfunctions for $-\mathbf{k}$ with the same energy $\varepsilon_{-\mathbf{k}}\,(=\varepsilon_{\mathbf{k}})$ are orthogonal:

$$\int \psi^{(1)}_{-\mathbf{k}}(\mathbf{r})^{+}\,\psi^{(2)}_{-\mathbf{k}}(\mathbf{r})\,d^3r = -i\int \left[u_{\mathbf{k}-}(\mathbf{r})\,u_{\mathbf{k}+}(-\mathbf{r}) - u_{\mathbf{k}+}(\mathbf{r})\,u_{\mathbf{k}-}(-\mathbf{r})\right]d^3r = 0\,. \tag{73}$$

Corollary: The Bloch-states (related to a given $\mathbf{k}$) of a nonmagnetic centro-symmetric crystal are at least twofold degenerate.

1.6 Sorting out the eigenstates by spin-expectation value

In general, the eigenfunctions $\psi_{\mathbf{k}}^{(\mu)}$ $(\mu = 1, 2)$ are not eigenfunctions of the spin-operator S_z for any chosen quantization axis z. This is only the case in the absence of spin-orbit coupling. Nevertheless, it is possible to construct the linear combinations,

$$\psi_{\mathbf{k}}^{(+)} = c_1 \psi_{\mathbf{k}}^{(1)} + c_2 \psi_{\mathbf{k}}^{(2)} \tag{74}$$

$$\psi_{\mathbf{k}}^{(-)} = -c_2^* \psi_{\mathbf{k}}^{(1)} + c_1^* \psi_{\mathbf{k}}^{(2)} \tag{75}$$

such that *(i)*

$$|c_1|^2 + |c_2|^2 = 1 \tag{76}$$

i.e. the two states are orthonormal, *(ii)*

$$\left\langle \psi_{\mathbf{k}}^{(+/-)} \left| \sigma_x \right| \psi_{\mathbf{k}}^{(+/-)} \right\rangle = \left\langle \psi_{\mathbf{k}}^{(+/-)} \left| \sigma_y \right| \psi_{\mathbf{k}}^{(+/-)} \right\rangle = 0 \tag{77}$$

and *(iii)*

$$\left\langle \psi_{\mathbf{k}}^{(+/-)} \left| \sigma_z \right| \psi_{\mathbf{k}}^{(+/-)} \right\rangle = \pm P\left(\mathbf{k}\right) \tag{78}$$

$$0 \leq P\left(\mathbf{k}\right) \leq 1 \tag{79}$$

Thus we can sort out the two degenerate states by the spectral spin-polarization, $P\left(\mathbf{k}\right)$. As it should apply for a nonmagnetic system, the expectation value of S_z within any eigen-subspace of the Hamiltonian is zero, since it always contains the orthonormal pairs of eigenfunctions, $\psi_{\mathbf{k}}^{(+)}$ and $\psi_{\mathbf{k}}^{(-)}$.

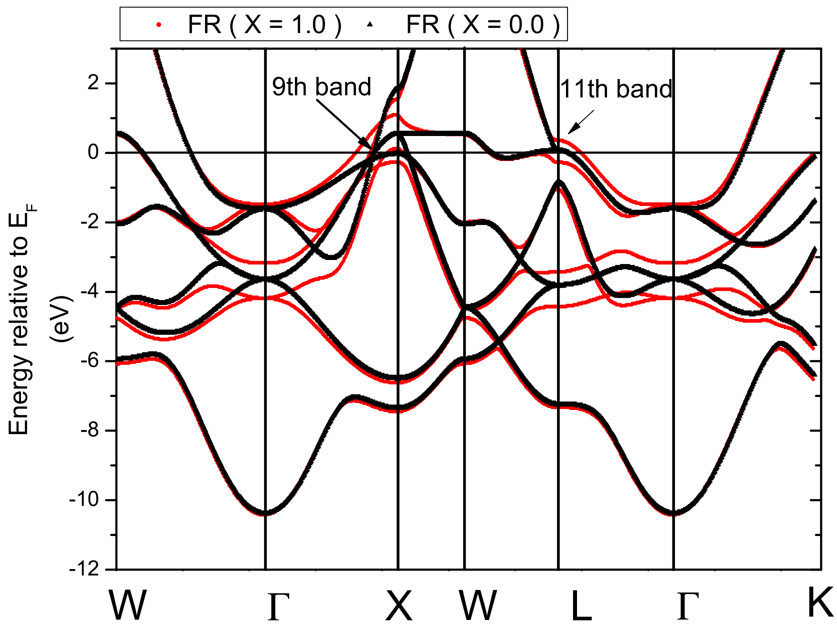

FIG. 2: Band structure of Pt from the fully relativistic (red) and the relativistic with the spin-orbit coupling scaled to zero (black) calculation.

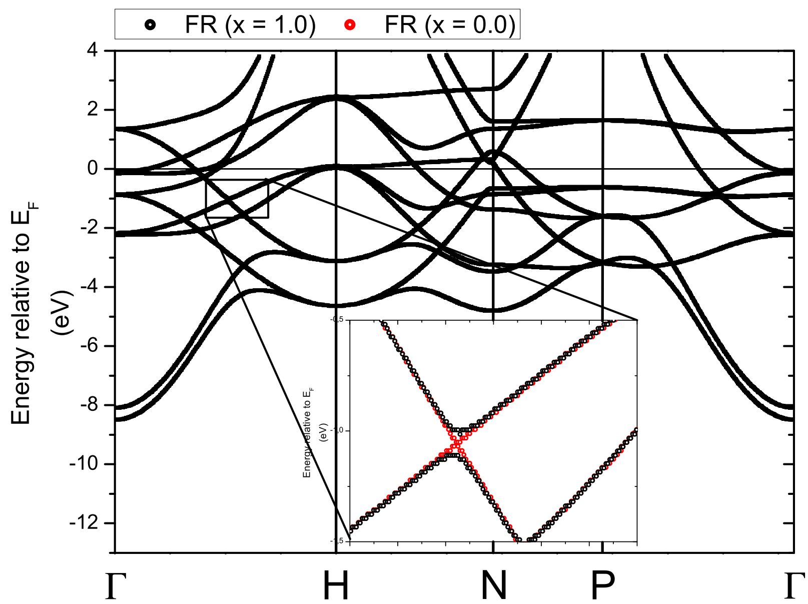

FIG. 3: Calculated fully relativistic band structure of bcc Fe. The small inset shows a comparison to the calculation with the spin-orbit coupling scaled to zero (x=0). The spin-orbit interaction leads to avoided crossings.

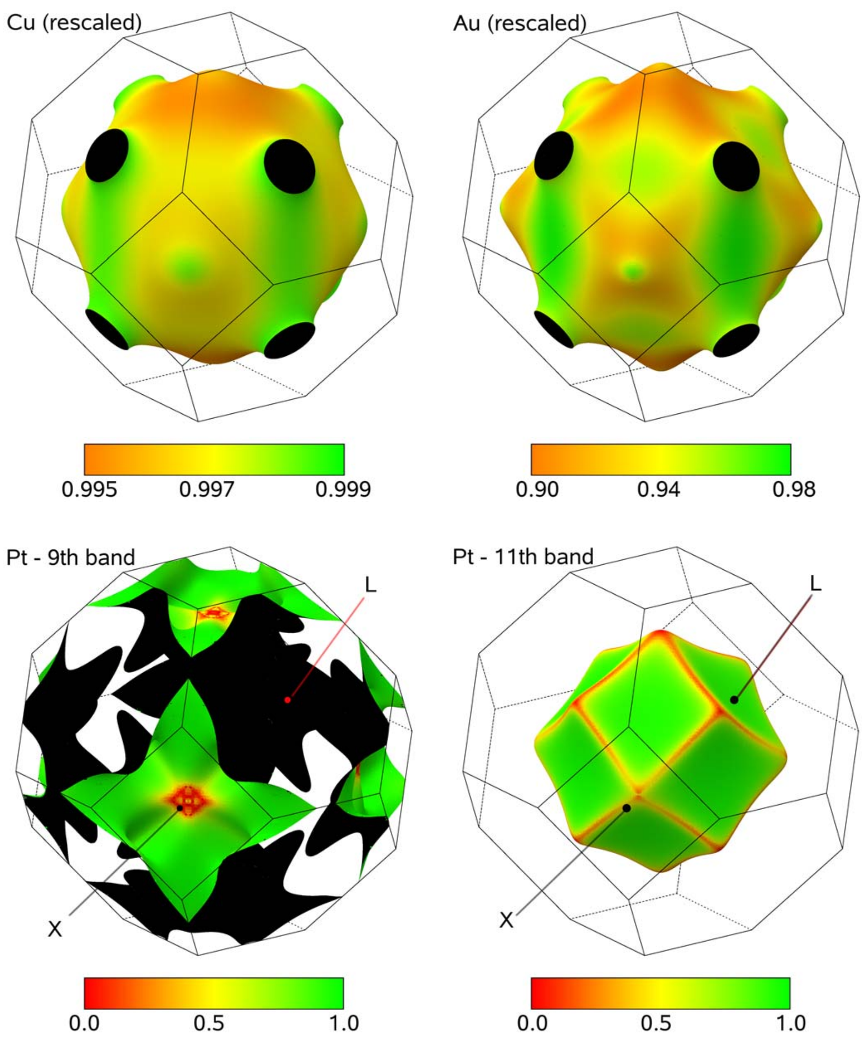

FIG. 4: Calculated relativistic Fermi surface of Cu (upper left), Au (upper right) and Pt (lower left: 9th band, lower right: 11th band), and the expectation values of $\hat{\beta}\sigma_z$ for the $\left|\Psi_k^+\right\rangle$ states are indicated as color code. Note the different scale for Cu and Au in comparison to Pt.

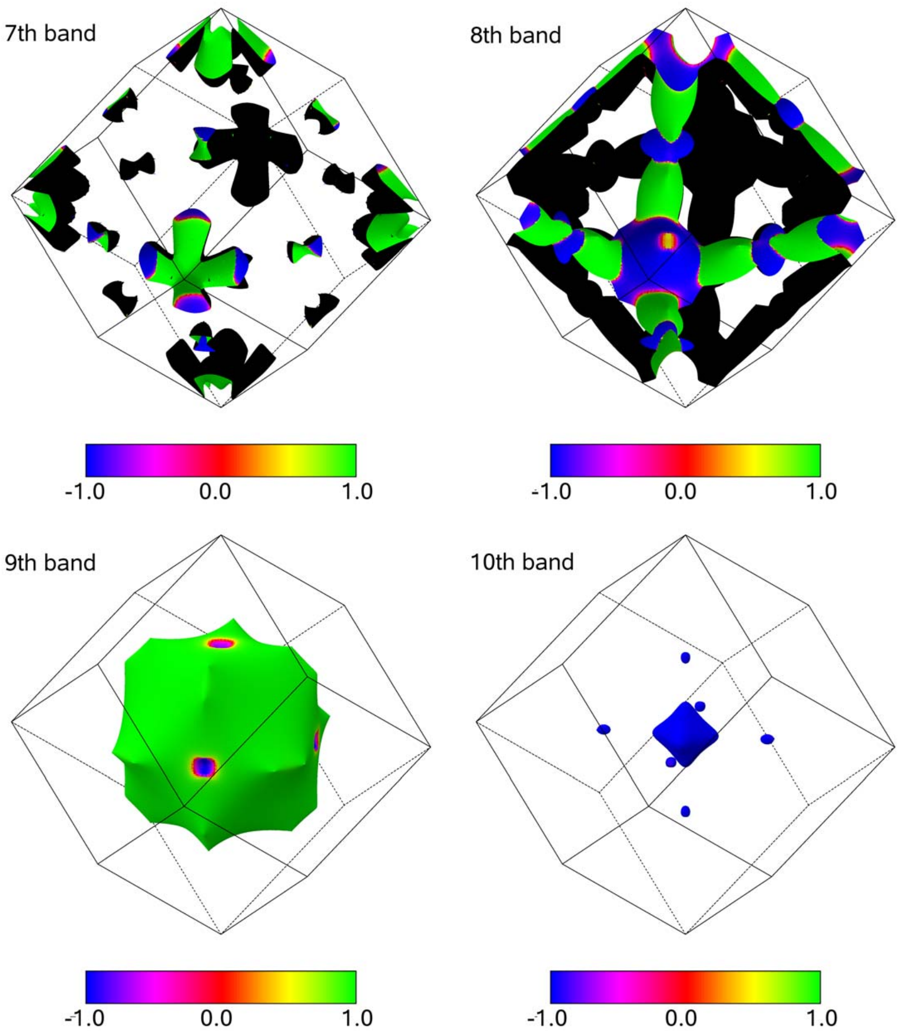

FIG. 5: Calculated relativistic Fermi surface for the bands 7-10 of bcc Fe. The expectation values of the $\hat{\beta}\sigma_z$ operator are given as color code.