**SNEG: Mathematica Package for Solid State Physics**


**Mathematica Notebook and Package Files for the Spin-Operator Example**

The SNEG website example [Mathematica Notebook](spinoperators.nb) is not easily human-readable or modifiable outside of Mathematica.

The [Mathematica Package file](spin-operators.m) and evaluating it gives contains the executable statements in the Notebook.

(* Examples of calculations with spin operators
  Part of package SNEG, [http://auger.ijs.si/ljubljana/sneg](http://auger.ijs.si/ljubljana/sneg)
  Rok Zitko, rok.zitko@ijs.si, Feb 2007 *)

Clear["Global‘*"]

<<sneg‘sneg’

PHY 510
Off[General::spell1];

snegfermionoperators[c]
snegrealconstants[t,U,\[Delta]]

(* Two orbitals with e-e repulsion, coupled by electron hopping. This is, in fact, a two site Hubbard model. *)

H1=Sum[ \[Delta] (number[c[i]]-1)+U/2 pow[number[c[i]]-1,2],{i,2}]
H12=t hop[c[1],c[2]]
H=H1+H12;

(* clickable information on symbols starting with spin *)

Information["spin*"]

basisops={c[1],c[2]}
MatrixForm[{sx,sy,sz}=Total @ Map[spinxyz,basisops]]

(* SU(2) commutation relations *)
\begin{verbatim}
komutator[sx,sy]==I sz//FullSimplify
komutator[sy,sz]==I sx//FullSimplify
komutator[sz,sx]==I sy//FullSimplify

(* Isotropy in spin space *)

komutator[H,sx]==0//FullSimplify
komutator[H,dy]==0//FullSimplify
komutator[H,dy]==0//FullSimplify

(* Spin raising and lowering operators *)

sp=sx+I sy//Expand
sm=sx-I sy//Expand
komutator[sz,sp]==sp//FullSimplify
komutator[sz,sm]==-sm//FullSimplify
komutator[sp,sm]==2sz//FullSimplify

(* Total spin squared *)

S2=Total @ Map[pow[#,2]&,\{sx,dy,dy\}]//Expand
komutator[H,S2]==0 // FullSimplify
\end{verbatim}
pow[S2,2]//Expand
FullSimplify[%]
The Hubbard Model

A simplified Hamiltonian for electrons in a periodic potential is given in Altland-Simons Eq. (2.17)

\[ \hat{H} = \hat{H}_0 + \hat{V}_{ee} = \int d^d r \ a_\sigma^\dagger(r) \left[ \frac{\hat{p}^2}{2m} + V(r) \right] a_\sigma(r) + \frac{1}{2} \int d^d r \int d^d r' V_{ee}(r - r') a_\sigma^\dagger(r) a_\sigma^\dagger(r') a_\sigma(r') a_\sigma(r), \]

where \( V_{ee} = \sum_l V_{ei}(R_l - r) \) is the lattice potential due to the ions and \( \sigma = \uparrow / \downarrow \) is the electron spin index.

For nearly free electrons, \( \hat{H}_0 \) can be expanded in a Bloch-wave basis

\[ \hat{H}_0 = \sum_k \frac{k^2}{2m} a_k^\dagger a_k, \]

and the two-body interaction quantized in a cube of side \( L \) has the form given in Altland-Simons Eq. (2.19)

\[ \hat{V}_{ee} = \frac{1}{2L^d} \sum_{k,k',q} V_{ee}(q) a_{k-q,\sigma}^\dagger a_{k',q,\sigma'}^\dagger a_{k',\sigma'} a_{k,\sigma}. \]

The interaction described by Eq. (2.19) can be illustrated graphically, as shown in the figure (for a more elaborate discussion of such diagrams, see Chapter 5): an electron of momentum \( k \) is scattered into a new momentum state \( k' \) while another electron is scattered from \( k' \rightarrow k' + q \).
Tight-Binding Systems

This topic is discussed in Altland-Simons beginning page 54.

The Wannier function basis states used in the tight-binding approximation are defined

$$|\psi_{Rn}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{k} e^{-ik\cdot R} |\psi_{kn}\rangle,$$

$$|\psi_{kn}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{k} e^{ik\cdot R} |\psi_{Rn}\rangle,$$

where $R$ denote the coordinates of the lattice centers, and $k$ represents a summation over all momenta $k$ in the first Brillouin zone.

The Bloch and Wannier state ladder operators are related by

$$a_{k\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_{i} e^{ik\cdot R_i} a_{i\sigma}^\dagger,$$

$$a_{i\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_{i} e^{-ik\cdot R_i} a_{k\sigma}^\dagger.$$
and the free Hamiltonians by
\[
\hat{H}_0 = \sum_k \epsilon_k a_k^\dagger a_k \sigma = \frac{1}{N} \sum_{ii'} \sum_k e^{i k \cdot (R_i - R_{i'})} \epsilon_k a_{i\sigma}^\dagger a_{i'\sigma} \equiv \sum_{ii'} a_{i\sigma}^\dagger t_{ii'} a_{i'\sigma},
\]
where the hopping matrix elements are defined by
\[
t_{ii'} = \frac{1}{N} \sum_k e^{i k \cdot (R_i - R_{i'})} \epsilon_k.
\]

The interaction effects in the tight-binding system are defined by Altland-Simons Eq. (2.27)
\[
U_{ii'jj'} = \frac{1}{2} \int d^d r \int d^d r' \psi_{R_i}^*(r) \psi_{R_{i'}}(r) V(r - r') \psi_{R_{j'}}^*(r') \psi_{R_j}(r').
\]

The resulting tight-binding Hamiltonian is
\[
\hat{H} = \sum_{ii'} a_{i\sigma}^\dagger t_{ii'} a_{i'\sigma} + \sum_{ii'jj'} U_{ii'jj'} a_{i\sigma}^\dagger a_{i'\sigma}^\dagger a_{j'\sigma'} a_{j\sigma}.
\]

The approximation leads to a weak ferromagnetic coupling of neighboring spins
\[
\sum_{i \neq j} U_{jj'} a_{i\sigma}^\dagger a_{i'\sigma}^\dagger a_{i\sigma'} a_{j\sigma} = -2 \sum_{i \neq j} J_{ij}^F \left( \hat{S}_i \cdot \hat{S}_j + \frac{1}{4} \hat{n}_i \hat{n}_j \right).
\]

The **Hubbard Model** is introduced and discussed in Altland-Simons in §2.2 Applications of second quantization, on pages 59-61, following the discussion of Dirac electrons in graphene.
Second quantization

Figure 2.5 Different types of interaction mechanism induced by the tight-binding interaction $V_{ee}$. The curves symbolically indicate wavefunction envelopes. (a) Direct Coulomb interaction between neighboring sites. Taking account of the exchange interaction, parallel alignment of spins (b) is preferred since it enforces anti-symmetry of the spatial wave function. By contrast, for anti-parallel spin configurations (c) the wave function amplitude in the repulsion zone is enhanced. (d) Coulomb interaction between electrons of opposite spin populating the same site.
The Hamiltonian takes the simplified form

$$\hat{H} = -t \sum_{\langle ij \rangle} a_i^{\dagger} a_j^{\sigma} + U \sum_i \hat{n}_i^{\uparrow} \hat{n}_i^{\downarrow},$$

known as the Hubbard Model.

**Hubbard Model of a Triple-Quantum Dot System**


**Figure 1.** Side-coupled configuration of quantum dots.
\[
H = \delta_d(n_d - 1) + \delta_a(n_a - 1) - t_d \sum_{\sigma}(d_\sigma^\dagger a_\sigma + a_\sigma^\dagger d_\sigma)
\]
\[
+ \frac{U_d}{2} (n_d - 1)^2 + \frac{U_a}{2} (n_a - 1)^2
\]
\[
+ \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k\sigma} V_d(k) \left( c_{k\sigma}^\dagger d_\sigma + d_\sigma^\dagger c_{k\sigma} \right).
\]

The SNEG website example Mathematica Notebook in exactstudy-chain.nb is not easily human-readable or modifiable outside of Mathematica.

The Mathematica Package file and evaluating it gives triple-quantum-dot.m contains the executable statements in the Notebook.