Exercises FYS4480, week 34, August 19-23, 2024

The exercises this week are mainly meant as reminders of specific linear algebra elements which we will use throughout the course.

Exercise 1, unitary transformations and orthogonality

In many-body theories it is common to expand a new basis interms of a known basis. Well-known examples thereof are the analytical solutions to the quantum mechanical harmonic oscillator or the atomic hydrogen case with a Coulomb interaction between the electron and the atomic nucleus. Varying the expansion coefficients leads then to a variational minimum which is expected to be closer to the true minimum, the so-called energy ground state (or fundamental state) of a system for a given Hamiltonian. This forms for example the background for mean-field theories, full configuration interaction theory and many other many-body methods. Normally these expansion coefficients represent the matrix elements of a unitary or orthogonal matrix.

Assuming that the matrix $\boldsymbol{U}$ is unitary with dimension $n \times n$ and matrix elements u_{ij}, we can, using a so-called Dirac notation for vectors, represent a new vector $|\psi_p\rangle$ of length n via another vector $|\phi_\lambda\rangle$ with length n through

$$|\psi_p\rangle = \boldsymbol{U}|\phi_\lambda\rangle.$$

It is common to assume that the basis vectors $|\phi\rangle$ are normalized and orthogonal and are the eigenvectors of an eigenvalue problem

$$\boldsymbol{O}|\phi_\lambda\rangle = o_\lambda|\phi_\lambda\rangle,$$

where $\boldsymbol{O}$ is a Hermitian matrix of dimension $n \times n$ and $_\lambda$ one of the n eigenvalues.

We have thus defined our new basis by performing a unitary (or othogonal) transformation as indicated in the first equation above.

a) Write down the properties of unitary and orthogonal matrices.

b) Write down the properties of hermitian matrices.

c) Assuming that the coefficients $u_{p\lambda}$ belong to a unitary or orthogonal trasformation, show that the new basis is orthogonal and normalized as well.

d) Show that the eigenvalues of $|\psi_p\rangle$ are the same as those of $|\phi_\lambda\rangle$.

Exercise 2, determinamts

a) Consider the following determinant

$$\left| \begin{array}{cc} \alpha_1 b_{11} + \alpha_2 s b_{12} & a_{12} \\ \alpha_1 b_{21} + \alpha_2 b_{22} & a_{22} \end{array} \right| = \alpha_1 \left| \begin{array}{cc} b_{11} & a_{12} \\ b_{21} & a_{22} \end{array} \right| + \alpha_2 \left| \begin{array}{cc} b_{12} & a_{12} \\ b_{22} & a_{22} \end{array} \right|$$

We can generalize this to an $n \times n$ matrix and have

$$\left| \begin{array}{cccccc} a_{11} & a_{12} & \dots & \sum_{k=1}^n c_k b_{1k} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & \sum_{k=1}^n c_k b_{2k} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & \sum_{k=1}^n c_k b_{nk} & \dots & a_{nn} \end{array} \right| = \sum_{k=1}^n c_k \left| \begin{array}{cccccc} a_{11} & a_{12} & \dots & b_{1k} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & b_{2k} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & b_{nk} & \dots & a_{nn} \end{array} \right|.$$

This is a property we will use in for example our discussions of mean-field theories.

Show that you can generalize the previous results, now with all elements a_{ij} being given as functions of linear combinations of various coefficients c and elements b_{ij},

$$\left| \begin{array}{cccccc} \sum_{k=1}^{n} b_{1k}c_{k1} & \sum_{k=1}^{n} b_{1k}c_{k2} & \dots & \sum_{k=1}^{n} b_{1k}c_{kj} & \dots & \sum_{k=1}^{n} b_{1k}c_{kn} \\ \sum_{k=1}^{n} b_{2k}c_{k1} & \sum_{k=1}^{n} b_{2k}c_{k2} & \dots & \sum_{k=1}^{n} b_{2k}c_{kj} & \dots & \sum_{k=1}^{n} b_{2k}c_{kn} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \sum_{k=1}^{n} b_{nk}c_{k1} & \sum_{k=1}^{n} b_{nk}c_{k2} & \dots & \sum_{k=1}^{n} b_{nk}c_{kj} & \dots & \sum_{k=1}^{n} b_{nk}c_{kn} \end{array} \right| = det(\mathbf{C})det(\mathbf{B}),$$

where $det(\mathbf{C})$ and $det(\mathbf{B})$ are the determinants of $n \times n$ matrices with elements c_{ij} and b_{ij} respectively.

b) With our definition from the previous exercise of the new basis in terms of an orthogonal basis we have (now we specialize to a specific basis of single-particle functions)

$$\psi_p(x) = \sum_{\lambda} C_{p\lambda}\phi_{\lambda}(x).$$

If the coefficients $C_{p\lambda}$ belong to an orthogonal or unitary matrix, the new basis is also orthogonal.

Show that the determinant in the new basis $\psi_p(x)$ can be written as (omitting a factor $1/\sqrt{N!}$, where N is the number of particles),

$$\left| \begin{array}{ccccc} \psi_p(x_1) & \psi_p(x_2) & \dots & \dots & \psi_p(x_N) \\ \psi_q(x_1) & \psi_q(x_2) & \dots & \dots & \psi_q(x_N) \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \psi_t(x_1) & \psi_t(x_2) & \dots & \dots & \psi_t(x_N) \end{array} \right| = \left| \begin{array}{ccccc} \sum_{\lambda} C_{p\lambda}\phi_{\lambda}(x_1) & \sum_{\lambda} C_{p\lambda}\phi_{\lambda}(x_2) & \dots & \dots & \sum_{\lambda} C_{p\lambda}\phi_{\lambda}(x_N) \\ \sum_{\lambda} C_{q\lambda}\phi_{\lambda}(x_1) & \sum_{\lambda} C_{q\lambda}\phi_{\lambda}(x_2) & \dots & \dots & \sum_{\lambda} C_{q\lambda}\phi_{\lambda}(x_N) \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \sum_{\lambda} C_{t\lambda}\phi_{\lambda}(x_1) & \sum_{\lambda} C_{t\lambda}\phi_{\lambda}(x_2) & \dots & \dots & \sum_{\lambda} C_{t\lambda}\phi_{\lambda}(x_N) \end{array} \right|,$$

which is nothing but $det(\mathbf{C})det(\Phi)$, with $det(\Phi)$ being the determinant given by the basis functions $\phi_{\lambda}(x)$.

c) Show that the new determinant (left hand side) differs from $det(\Phi)$ by a complex phase only.