

Exercises FYS4480, week 34, August 18-22, 2025

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 in terms 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 \mathbf{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

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

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

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

where \mathbf{O} is a Hermitian matrix of dimension $n \times n$ and λ one of the n eigenvalues.

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

- Write down the properties of unitary and orthogonal matrices.
- Write down the properties of hermitian matrices.
- Assuming that the coefficients $u_{p\lambda}$ belong to a unitary or orthogonal transformation, show that the new basis is orthogonal and normalized as well.
- Show that the eigenvalues of $|\psi_p\rangle$ are the same as those of $|\phi_\lambda\rangle$.

Exercise 2, determinants

- Consider the following determinant

$$\begin{vmatrix} \alpha_1 b_{11} + \alpha_2 b_{12} & a_{12} \\ \alpha_1 b_{21} + \alpha_2 b_{22} & a_{22} \end{vmatrix} = \alpha_1 \begin{vmatrix} b_{11} & a_{12} \\ b_{21} & a_{22} \end{vmatrix} + \alpha_2 \begin{vmatrix} b_{12} & a_{12} \\ b_{22} & a_{22} \end{vmatrix}$$

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

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

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} ,

$$\begin{vmatrix} \sum_{k=1}^n b_{1k}c_{k1} & \sum_{k=1}^n b_{1k}c_{k2} & \cdots & \sum_{k=1}^n b_{1k}c_{kj} & \cdots & \sum_{k=1}^n b_{1k}c_{kn} \\ \sum_{k=1}^n b_{2k}c_{k1} & \sum_{k=1}^n b_{2k}c_{k2} & \cdots & \sum_{k=1}^n b_{2k}c_{kj} & \cdots & \sum_{k=1}^n b_{2k}c_{kn} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \sum_{k=1}^n b_{nk}c_{k1} & \sum_{k=1}^n b_{nk}c_{k2} & \cdots & \sum_{k=1}^n b_{nk}c_{kj} & \cdots & \sum_{k=1}^n b_{nk}c_{kn} \end{vmatrix} = \det(\mathbf{C})\det(\mathbf{B}),$$

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),

$$\begin{vmatrix} \psi_p(x_1) & \psi_p(x_2) & \cdots & \cdots & \psi_p(x_N) \\ \psi_q(x_1) & \psi_q(x_2) & \cdots & \cdots & \psi_q(x_N) \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \psi_t(x_1) & \psi_t(x_2) & \cdots & \cdots & \psi_t(x_N) \end{vmatrix} = \begin{vmatrix} \sum_{\lambda} C_{p\lambda} \phi_{\lambda}(x_1) & \sum_{\lambda} C_{p\lambda} \phi_{\lambda}(x_2) & \cdots & \cdots & \sum_{\lambda} C_{p\lambda} \phi_{\lambda}(x_N) \\ \sum_{\lambda} C_{q\lambda} \phi_{\lambda}(x_1) & \sum_{\lambda} C_{q\lambda} \phi_{\lambda}(x_2) & \cdots & \cdots & \sum_{\lambda} C_{q\lambda} \phi_{\lambda}(x_N) \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \sum_{\lambda} C_{t\lambda} \phi_{\lambda}(x_1) & \sum_{\lambda} C_{t\lambda} \phi_{\lambda}(x_2) & \cdots & \cdots & \sum_{\lambda} C_{t\lambda} \phi_{\lambda}(x_N) \end{vmatrix},$$

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.