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 using a known basis and vary the expansion coefficients. Normally these expansion coefficients represent the matrix elements of a unitary or orthogonal matrix.

We define our new basis by performing a unitary transformation on our original orthogonal and normalized (orthonormal for short) basis, labelled with greek indices and with a Dirac notation, as

$$|\psi_p\rangle = \sum_\lambda C_{p\lambda}|\phi_\lambda\rangle.$$

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

Exercise 2, determinamts

a) Consider the following determinant

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

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},

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

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 (with a factor $1/\sqrt{N!}$, where N is the number of particles,

$$
\frac{1}{\sqrt{N!}}
\begin{vmatrix}
\psi_p(x_1) & \psi_p(x_2) & \dots & \dots & \psi_p(x_N) \\
\psi_q(x_1) & \psi_q(x_2) & \dots & \dots & \psi_q(x_N) \\
\dots & \dots & \dots & \dots & \dots \\
\dots & \dots & \dots & \dots & \dots \\
\psi_t(x_1) & \psi_t(x_2) & \dots & \dots & \psi_t(x_N)
\end{vmatrix}
=
\frac{1}{\sqrt{N!}}
\begin{vmatrix}
\sum_\lambda C_{p\lambda}\phi_\lambda(x_1) & \sum_\lambda C_{p\lambda}\phi_\lambda(x_2) & \dots & \dots & \sum_\lambda C_{p\lambda}\phi_\lambda(x_N) \\
\sum_\lambda C_{q\lambda}\phi_\lambda(x_1) & \sum_\lambda C_{q\lambda}\phi_\lambda(x_2) & \dots & \dots & \sum_\lambda C_{q\lambda}\phi_\lambda(x_N) \\
\dots & \dots & \dots & \dots & \dots \\
\dots & \dots & \dots & \dots & \dots \\
\sum_\lambda C_{t\lambda}\phi_\lambda(x_1) & \sum_\lambda C_{t\lambda}\phi_\lambda(x_2) & \dots & \dots & \sum_\lambda C_{t\lambda}\phi_\lambda(x_N)
\end{vmatrix},
$$

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 differs from $det(\Phi)$ by a complex phase only.