

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, determinants

a) 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} ,

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

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

$$\begin{array}{c} \overline{\psi_p(x_1)} \quad \overline{\psi_p(x_2)} \quad \dots \quad \overline{\psi_p(x_N)} \\ \overline{\psi_q(x_1)} \quad \overline{\psi_q(x_2)} \quad \dots \quad \overline{\psi_q(x_N)} \\ \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \\ \overline{\psi_t(x_1)} \quad \overline{\psi_t(x_2)} \quad \dots \quad \overline{\psi_t(x_N)} \end{array} \bigg| \overset{1}{=} \begin{array}{c} \sum_{\lambda} C_{p\lambda} \phi_{\lambda}(x_1) \quad \sum_{\lambda} C_{p\lambda} \phi_{\lambda}(x_2) \quad \dots \quad \sum_{\lambda} C_{p\lambda} \phi_{\lambda}(x_N) \\ \sum_{\lambda} C_{q\lambda} \phi_{\lambda}(x_1) \quad \sum_{\lambda} C_{q\lambda} \phi_{\lambda}(x_2) \quad \dots \quad \sum_{\lambda} C_{q\lambda} \phi_{\lambda}(x_N) \\ \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \\ \sum_{\lambda} C_{t\lambda} \phi_{\lambda}(x_1) \quad \sum_{\lambda} C_{t\lambda} \phi_{\lambda}(x_2) \quad \dots \quad \sum_{\lambda} C_{t\lambda} \phi_{\lambda}(x_N) \end{array} \bigg|,$$

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.