Advanced Quantum Mechanics
Exercise Series 8

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Exercise 19

Let $n \in \mathbb{N}$ be a natural number, $A \in \mathbb{R}^{n\times n}$ with $A^{\mathrm{T}} = A$ a symmetric real matrix and $\langle \cdot, \cdot \rangle$ be the dot product on $\mathbb{R}^n$. Using the spectral theorem, we know that there exists an orthonormal basis $\mathcal{B} := \{b_i \in \mathbb{R}^n \mid i \in \mathbb{N}, i \leq n\}$ such that b is an eigenvector of A for all $b \in \mathcal{B}$. It is now convenient to define the following orthogonal matrix $S \in \mathbb{R}^{n\times n}$.

$$S := (b_1, \ldots, b_n)$$

Because S is an orthogonal matrix, we can conclude the following propositions.

$$\det S = \pm 1, \quad S^{\mathrm{T}}S = SS^{\mathrm{T}} = \mathrm{I}$$

Additionally, we define $\lambda_i \in \mathbb{R}$ with $Ab_i = \lambda_i b_i$ as the eigenvalue of the i.basis-vector for all $i \in \mathbb{N}$ with $i \leq n$. Of course, these eigenvalues do not have to be distinct. Using $\langle b_i, b_j \rangle = \delta_{ij}$ for all $i, j \in \mathbb{N}$ with $i, j \leq n$ we get the following result.

$$\begin{aligned}
\tilde{A} := S^{\mathrm{T}}AS &= (b_1, \ldots, b_n)^{\mathrm{T}} A (b_1, \ldots, b_n) \\
&= (b_1, \ldots, b_n)^{\mathrm{T}} (Ab_1, \ldots, Ab_n) \\
&= (b_1, \ldots, b_n)^{\mathrm{T}} (\lambda_1 b_1, \ldots, \lambda_n b_n) \\
&= \mathrm{diag}\,(\lambda_1, \ldots, \lambda_n)
\end{aligned}$$

$\tilde{A}$ is a diagonal matrix. Hence, the determinants of A and $\tilde{A}$ are given by the product of all eigenvalues of A.

$$\det A = \det \tilde{A} = \prod_{k=1}^{n} \lambda_k$$

We apply this result to the the functions $f, \tilde{f} \colon \mathbb{R}^n \to \mathbb{C}$ with the following definitions for all $x \in \mathbb{R}^n$.

$$f(x) := \exp\left(\frac{\mathrm{i}}{2\hbar} \langle x, Ax \rangle\right)$$

$$\tilde{f}(x) := \exp\left(\frac{\mathrm{i}}{2\hbar} \left\langle x, \tilde{A}x \right\rangle\right)$$

By using the bijective function $\varphi \colon \mathbb{R}^n \to \mathbb{R}^n$ with $\varphi(x) := S^{\mathrm{T}}x$ for all $x \in \mathbb{R}^n$, we get the following.

$$\begin{aligned}
f(x) &= \exp\left(\frac{\mathrm{i}}{2\hbar} \left\langle SS^{\mathrm{T}}x, ASS^{\mathrm{T}}x \right\rangle\right) \\
&= \exp\left[\frac{\mathrm{i}}{2\hbar} \left\langle \left(S^{\mathrm{T}}x\right), S^{\mathrm{T}}AS\left(S^{\mathrm{T}}x\right) \right\rangle\right] \\
&= \exp\left(\frac{\mathrm{i}}{2\hbar} \left\langle \varphi(x), \tilde{A}\varphi(x) \right\rangle\right) \\
&= \tilde{f} \circ \varphi(x)
\end{aligned}$$

Now we have to rearrange the explicit form of $\tilde{f}(x)$ for all $x \in \mathbb{R}^n$ by using the definition of $\tilde{A}$.

$$\begin{aligned}
\tilde{f}(x) &= \exp\left(\frac{\mathrm{i}}{2\hbar} \langle x, \mathrm{diag}\,(\lambda_1, \ldots, \lambda_n)\, x \rangle\right) \\
&= \exp\left(\frac{\mathrm{i}}{2\hbar} \sum_{k=1}^{n} \lambda_k x_k^2\right) \\
&= \prod_{k=1}^{n} \exp\left(\frac{\mathrm{i}}{2\hbar} \lambda_k x_k^2\right)
\end{aligned}$$

Since $\mathbb{R}^n$ is an unbounded set and $|f| = \mathrm{id}$ we have $\int_{\mathbb{R}^n} |f| \,\mathrm{d}\lambda^n = \infty$ with λ^n as the n-dimensional Lebesgue-measure on $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n))$. Therefore the function f is not Lebesgue-integrable. We have to rely on the improper Riemann-integral. Using $\det \mathrm{D}\varphi(x) = \det S^{\mathrm{T}} = \pm 1$,the transformation theorem and the theorem of Fubini, we are able to cut down the actual calculation to a one-dimensional improper Riemann-integral over complex numbers.

$$\begin{aligned}
\int_{\mathbb{R}^n} f(x)\,\mathrm{d}^n x &= \int_{\mathbb{R}^n} \tilde{f}(\varphi(x))\,\mathrm{d}^n x \\
&= \int_{\mathbb{R}^n} \tilde{f}(\varphi(x))\,|\det \mathrm{D}\varphi(x)|\,\mathrm{d}^n x \\
\text{(transformation)} &= \int_{\varphi(\mathbb{R}^n)} \tilde{f}(y)\,\mathrm{d}^n y \\
&= \int_{\mathbb{R}^n} \prod_{k=1}^{n} \exp\left(\frac{\mathrm{i}}{2\hbar}\lambda_k y_k^2\right) \mathrm{d}^n y \\
\text{(Fubini theorem)} &= \prod_{k=1}^{n} \int_{-\infty}^{\infty} \exp\left(\frac{\mathrm{i}}{2\hbar}\lambda_k x^2\right) \mathrm{d}x \\
&= \prod_{k=1}^{n} 2\int_{0}^{\infty} \exp\left(\frac{-\lambda_k x^2}{2\mathrm{i}\hbar}\right) \mathrm{d}x
\end{aligned}$$

Because the improper Riemann-integral is not well-defined on the complete real axis, some problems may arise when using the transformation theorem on $\mathbb{R}^n$. We could circumvent these problems by observing the actual limits of the integral.

To evaluate the one-dimensional integrals one has to use Cauchy's theorem for holomorphic functions. For $k \in \mathbb{N}$, $k \leq n$ we define the following curves in $\mathbb{C}$.

$$\gamma_k \colon \mathbb{R}^+ \to \mathbb{C}, \quad \gamma_k(x) := \sqrt{\frac{\lambda_k}{2\mathrm{i}\hbar}}\,x$$

Using these curves together with the transformation theorem and the definition of line integrals, we achieve the following result.

$$\begin{aligned}
&\int_0^\infty \exp\left(\frac{-\lambda_k x^2}{2\mathrm{i}\hbar}\right)\,\mathrm{d}x \\
&\qquad= \int_0^\infty \exp\left(-\gamma_k^2(x)\right)\,\mathrm{d}x \\
&\qquad= \int_0^\infty \exp\left(-\gamma_k^2(x)\right)\frac{\gamma_k'(x)}{\gamma_k'(x)}\,\mathrm{d}x \\
&\qquad= \sqrt{\frac{2\mathrm{i}\hbar}{\lambda_k}}\int_{\gamma_k\left(\mathbb{R}^+\right)} e^{-z^2}\,\mathrm{d}\gamma_k(z)
\end{aligned}$$

This equation holds even if $\lambda_k = 0$. In this case this integral is evaluated to ∞.

Applying Cauchy's theorem on the sector-shaped region given by the direction of γ_k' and the x-axis with radius $R \in \mathbb{R}^+$, we obtain the following with $\tilde{R} \coloneqq |\gamma_k'|\,R$.

$$\begin{aligned}
&\int_0^R e^{-t^2}\,\mathrm{d}t - \int_{\gamma_k\left((0,\tilde{R})\right)} e^{-z^2}\,\mathrm{d}\gamma_k(z) \\
&\qquad\qquad + \underbrace{\int_0^{\arg\gamma_k'} e^{-R^2e^{2\mathrm{i}\vartheta}}\,\mathrm{d}\vartheta}_{\xrightarrow{R\to\infty} 0} = 0
\end{aligned}$$

As R goes to infinity, the equation becomes the following with the well known half Gaussian integral.

$$\int_{\gamma_k\left(\mathbb{R}^+\right)} e^{-z^2}\,\mathrm{d}\gamma_k(z) = \int_0^\infty e^{-t^2}\,\mathrm{d}t = \sqrt{\frac{\pi}{4}}$$

Putting everything together, we are now able to find the solution to the integral.

$$\begin{aligned}
\int_{\mathbb{R}^n} f(x)\,\mathrm{d}^n x &= \prod_{k=1}^n 2\int_0^\infty \exp\left(\frac{-\lambda_k x^2}{2\mathrm{i}\hbar}\right)\,\mathrm{d}x \\
&= \prod_{k=1}^n 2\sqrt{\frac{2\mathrm{i}\hbar}{\lambda_k}}\int_{\gamma_k\left(\mathbb{R}^+\right)} e^{-z^2}\,\mathrm{d}\gamma_k(z) \\
&= \prod_{k=1}^n \sqrt{\frac{8\mathrm{i}\hbar}{\lambda_k}}\int_0^\infty e^{-t^2}\,\mathrm{d}t \\
&= \prod_{k=1}^n \sqrt{\frac{2\mathrm{i}\pi\hbar}{\lambda_k}} = \frac{(2\mathrm{i}\pi\hbar)^{\frac{n}{2}}}{\sqrt{\prod_{k=1}^n \lambda_k}} \\
&= \frac{(2\mathrm{i}\pi\hbar)^{\frac{n}{2}}}{\sqrt{\det A}}
\end{aligned}$$

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