

Notes

Quantum Mechanics

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Caprice

1 Fall 2018

1.1 Derivation of I.2 (28) in Appendix 3

| Section 1. Fall 2018

To do an integral of form $I = \int_{-\infty}^{\infty} dq \exp[-f(x)/\hbar]$, we often have to resort to steepest-descent method. In limit of $\hbar \rightarrow 0$, the integral is dominated by the minimum of $f(a) = \min[f(q)]$, Expanding $f(q)$ around a

$$f(q) = f(a) + \frac{1}{2}f''(a)(q-a)^2 + \mathcal{O}[(q-a)^3] \quad (1.1)$$

This is a Gaussian integral

$$\begin{aligned} I &= \int_{-\infty}^{\infty} dq e^{-f(x)/\hbar} \\ &= e^{-f(a)/\hbar} \left[\frac{2\pi\hbar}{f''(a)} \right]^{\frac{1}{2}} e^{-\mathcal{O}(\hbar^{\frac{1}{2}})} \end{aligned}$$

Suppose now $f(\mathbf{q})$ is a function of multiple variables $\mathbf{q} = (q_1, \dots, q_N)$, then the expansion of $f(\mathbf{q})$ around the equilibrium position $\mathbf{a} = (a_1, \dots, a_N)$ can be written as

$$f(\mathbf{q}) = f(\mathbf{a}) + \frac{1}{2}(\mathbf{q} - \mathbf{a})^\top f''(\mathbf{a})(\mathbf{q} - \mathbf{a}) + \mathcal{O}[|\mathbf{q} - \mathbf{a}|^3] \quad (1.2)$$

where $f''(\mathbf{q})$ is understood as the Hessian of $f(\mathbf{q})$

$$[f''(\mathbf{q})]_{i,j} = \frac{\partial^2 f}{\partial q_i \partial q_j} \quad (1.3)$$

Therefore we rewrite the integral

$$\begin{aligned} I &= \int d\mathbf{q} e^{-f(\mathbf{q}/\hbar)} \\ &= e^{-f(\mathbf{a})/\hbar} \int d\mathbf{q} \exp \left[\frac{1}{2\hbar}(\mathbf{q} - \mathbf{a})^\top f''(\mathbf{a})(\mathbf{q} - \mathbf{a}) \right] e^{-\mathcal{O}(\hbar^{\frac{1}{2}})} \end{aligned}$$

where

$$\begin{aligned} &\exp \left[\frac{1}{2\hbar}(\mathbf{q} - \mathbf{a})^\top f''(\mathbf{a})(\mathbf{q} - \mathbf{a}) \right] \\ &= (\mathbf{q} - \mathbf{a})^\top \sum_{k=0}^{\infty} \frac{[f''(\mathbf{a})]^k}{k!(2\hbar)^k} (\mathbf{q} - \mathbf{a}) \\ &= (\mathbf{q} - \mathbf{a})^\top U^\top \sum_{k=0}^{\infty} \frac{[U f''(\mathbf{a}) U^\top]^k}{k!(2\hbar)^k} U (\mathbf{q} - \mathbf{a}) \\ &= \mathbf{y}^\top \exp[U f''(\mathbf{a}) U^\top / 2\hbar] \mathbf{y} \end{aligned}$$

where U is an orthogonal matrix such that $U^\top U = \mathbb{I}$, and $\mathbf{y} = U\mathbf{q}$. Choose U such that $U f''(\mathbf{a}) U^\top$ is a diagonal matrix, with the diagonal elements equal to its eigenvalues

$$[U f''(\mathbf{a}) U^\top]_{i,i} = \mu_i \quad (1.4)$$

Then

$$\mathbf{y}^\top \exp [U f''(\mathbf{a}) U^\top / 2\hbar] \mathbf{y} = \exp \left(\frac{1}{2\hbar} \sum_i \mu_i y_i^2 \right) \quad (1.5)$$

Under the change of variables, the differential elements $d\mathbf{q} \rightarrow d\mathbf{y} = |\frac{\partial \mathbf{y}}{\partial \mathbf{q}}| d\mathbf{q}$, so the Jacobian is $\det(U) = 1$. Eventually we get the product of Gaussian integrals

$$\begin{aligned} I &= \int d\mathbf{q} e^{-f(\mathbf{q}/\hbar)} \\ &= \int d\mathbf{y} \exp \left(\frac{1}{2\hbar} \sum_i \mu_i y_i^2 \right) \\ &= \prod_{i=1}^N \int_{-\infty}^{\infty} dy_i \left[\exp \left(\frac{1}{2\hbar} \mu_i y_i^2 \right) \right] \\ &= \left[\frac{(2\pi\hbar)^N}{\prod_i \mu_i} \right]^{\frac{1}{2}} = \left[\frac{(2\pi\hbar)^N}{\det[f''(\mathbf{a})]} \right]^{\frac{1}{2}} \end{aligned}$$