9 Response theory

Remark 9.1. In the presence of a time-varying field, a molecule's electronic wavefunction is no longer simply an eigenfunction of the Hamiltonian. Instead, its electronic structure is described by the *time-dependent Schrödinger equation*

$$H(t)\Psi(t) = i\frac{\partial\Psi(t)}{\partial t} \qquad H(t) = H + V(t) \tag{9.1}$$

where H is the usual electronic Hamiltonian and $V(t)$ is an *interaction Hamiltonian* describing the energetic influence of the field. A general series solution to equation 9.1, known as the *Dyson series*, is derived in appendix A. The interaction Hamiltonian can be expressed as a sum over one-electron operators V_β, representing the electronic degrees of freedom which couple to the external field, scaled by *time-envelopes* $f_\beta(t)$ which control the strength of the applied field over time.

$$V(t) = \textstyle\sum_\beta V_\beta f_\beta(t) \tag{9.2}$$

One of the most important examples is the Hamiltonian of a dipole in an electric field, which is discussed in ex 9.1 below. The zeroth order solutions of equation 9.1 are termed *stationary states*, which have the following form.[1]

$$\Psi(t)|_{\boldsymbol{f}=\mathbf{0}} = e^{-iE_k t}\Psi_k \qquad H\Psi_k = E_k\Psi_k \tag{9.3}$$

As a boundary condition we assume that $V(t)$ vanishes in the past, where $\Psi(t)$ is initially in the ground stationary state.

$$\lim_{t\to-\infty} f_\beta(t) = 0 \qquad \lim_{t\to-\infty} e^{+iHt}\Psi(t) = \Psi_0 \tag{9.4}$$

This limiting behavior can be enforced by introducing a complex shift in the frequency domain of $f_\beta(t)$'s Fourier expansion.[2]

$$f_\beta(t) = \int_{-\infty}^{\infty} d\omega\, f_\beta(\omega_\epsilon) e^{-i\omega_\epsilon t} \qquad f_\beta(\omega_\epsilon) \equiv (2\pi)^{-1}\int_{-\infty}^{\infty} dt\, f_\beta(t) e^{+i\omega_\epsilon t} \qquad \omega_\epsilon \equiv \omega + i\epsilon \qquad \epsilon = |\epsilon| \tag{9.5}$$

This has the effect of scaling the time envelope by a damping factor $e^{\epsilon t}$. For sufficiently small ϵ, this scaled envelope will match the original one to arbitrary precision in an arbitrarily wide window about the time origin. The fact that the interaction Hamiltonian and the coupling operators $\{V_\beta\}$ are Hermitian implies the following identities.

$$f_\beta^*(t) = f_\beta(t) \qquad f_\beta^*(\omega_\epsilon) = f_\beta(-\omega_{-\epsilon}) \tag{9.6}$$

Example 9.1. The dominant coupling of an electronic system to an external electric or magnetic field is mediated through its dipoles, leading to *the dipole approximation*. Quantizing the classical formulae for these interaction energies gives

$$\begin{array}{lll} V_{\mathbf{E}}(t) \approx -\boldsymbol{\mu}\cdot\mathbf{E}(t) = -\sum_\beta \mu_\beta \mathcal{E}_\beta(t) & \boldsymbol{\mu} = \sum_{pq}\langle\psi_p|\hat{\boldsymbol{\mu}}|\psi_q\rangle a_p^\dagger a_q & \hat{\boldsymbol{\mu}} = -\hat{\mathbf{r}} \\ V_{\mathbf{B}}(t) \approx -\boldsymbol{m}\cdot\mathbf{B}(t) = -\sum_\beta m_\beta \mathcal{B}_\beta(t) & \boldsymbol{m} = \sum_{pq}\langle\psi_p|\hat{\boldsymbol{m}}|\psi_q\rangle a_p^\dagger a_q & \hat{\boldsymbol{m}} = -\frac{1}{2}(\hat{\boldsymbol{l}} + 2\,\hat{\mathbf{s}}) \end{array} \tag{9.7}$$

where $\hat{\boldsymbol{\mu}}$ and $\hat{\boldsymbol{m}}$ are the first-quantized electric and magnetic dipole operators.[3] The leading terms neglected by the dipole approximation are quadratic in the field amplitudes. These weaker interactions are mediated through the higher moments (quadrupole, octupole, etc.) of the charge and current distributions and may become important in symmetric molecules where certain dipole interactions are "symmetry forbidden".

Definition 9.1. ***Quasi-energy.***

$$\Psi(t) = e^{-i\theta(t)}\bar{\Psi}(t) \qquad \theta(t)|_{\boldsymbol{f}=\mathbf{0}} = E_0 t \qquad \lim_{t\to-\infty}\bar{\Psi}(t) = \Psi_0 \tag{9.8}$$

$$(H(t) - i\tfrac{\partial}{\partial t})\bar{\Psi}(t) = \dot{\theta}(t)\bar{\Psi}(t) \tag{9.9}$$

$$\dot{\theta}(t) = \int_0^t dt'\langle\bar{\Psi}(t')|H(t') - i\tfrac{\partial}{\partial t'}|\bar{\Psi}(t')\rangle \tag{9.10}$$

$$\langle\delta\bar{\Psi}(t)|H(t) - i\tfrac{\partial}{\partial t}|\bar{\Psi}(t)\rangle = \dot{\theta}(t)\langle\delta\bar{\Psi}(t)|\bar{\Psi}(t)\rangle \tag{9.11}$$

$$\langle\delta\bar{\Psi}(t)|\bar{\Psi}(t)\rangle + \langle\bar{\Psi}(t)|\delta\bar{\Psi}(t)\rangle = 0 \tag{9.12}$$

$$\delta\langle\bar{\Psi}(t)|H(t) - i\tfrac{\partial}{\partial t}|\bar{\Psi}(t)\rangle + i\tfrac{\partial}{\partial t}\langle\bar{\Psi}(t)|\delta\bar{\Psi}(t)\rangle = 0 \tag{9.13}$$

---

[1] When $\boldsymbol{f} = \mathbf{0}$, the Hamiltonian loses its time-dependence and we can write $\Psi(t)|_{\boldsymbol{f}=\mathbf{0}} = \phi(t)\Psi$ where $\phi(t)$ is independent of the electronic coordinates. Substituting this into eq 9.1 and rearranging gives $H\Psi/\Psi = i\dot{\phi}(t)/\phi(t)$, which equals a constant E since each side depends in different variables. Therefore, $H\Psi = E\Psi$ and $i\dot{\phi}(t) = E\phi(t)$. Integrating the latter gives $\phi(t) = e^{-iEt}$.

[2] This is a slightly unusual convention for the Fourier transform. A useful mnemonic for checking these is $\int_{-\infty}^{\infty} dk\, e^{ikx} = 2\pi\,\delta(x)$.

[3] More generally, these expressions are $\hat{\boldsymbol{\mu}} = q_e\,\hat{\mathbf{r}}$, where $q_e = -e$ is the charge of an electron, and $\hat{\boldsymbol{m}} = \mu_{\mathrm{B}}(g_l\,\hat{\boldsymbol{l}} + g_{\mathrm{s}}\,\hat{\mathbf{s}})$ where $\mu_{\mathrm{B}} = \frac{1}{2}\cdot\frac{e\hbar}{m_e}$ is the Bohr magneton and $g_l = -1$, $g_{\mathrm{s}} = -2$ are the spin and orbital *g-factors*. Note that the exact g_{s} actually deviates very slightly from 2 due to effects arising in quantum field theory. The orbital angular momentum operator is given by $\hat{\boldsymbol{l}} = \hat{\mathbf{r}}\times\hat{\mathbf{p}}$ and $\hat{\mathbf{s}}$ is the intrinsic spin angular momentum operator.

A Dyson series

Definition A.1. ***Time-evolution operator.*** If we know the wavefunction at a particular time t_0, we can express the wavefunction at any other time as a unitary transformation of this initial state, $\Psi(t) = U(t,t_0)\Psi(t_0)$. This unitary transformation is called the *time-evolution operator*.

Definition A.2. ***Interaction picture.*** The *interaction picture* results from to the following similarity transformation.

$$\tilde{\Theta}(t) \equiv e^{+iHt}\Theta(t) \qquad \tilde{W}(t) \equiv e^{+iHt}W(t)e^{-iHt} \tag{A.1}$$

Expanding the Schrödinger equation in the interaction picture yields the the *Schwinger-Tomonaga equation*.

$$\tilde{V}(t)\tilde{\Psi}(t) = i\frac{\partial\tilde{\Psi}(t)}{\partial t} \tag{A.2}$$

Multiplying both sides by $-i$ and integrating from t_0 to t yields a recursive equation for the time-evolution operator

$$\tilde{\Psi}(t) - \tilde{\Psi}(t_0) = -i\int_{t_0}^{t} dt'\,\tilde{V}(t')\tilde{\Psi}(t') \qquad \Longrightarrow \qquad \tilde{U}(t,t_0) = 1 - i\int_{t_0}^{t} dt'\tilde{V}(t')\,\tilde{U}(t',t_0) \tag{A.3}$$

and infinite recursion of this identity leads to the following expansion.

$$\tilde{U}(t,t_0) = \sum_{n=0}^{\infty}(-i)^n\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\cdots\int_{t_0}^{t_{n-1}}dt_n\,\tilde{V}(t_1)\cdots\tilde{V}(t_n) \tag{A.4}$$

Definition A.3. ***Time-ordering.*** Let $\tilde{q}_1(t_1)\cdots\tilde{q}_n(t_n)$ be a string of particle-hole operators in the interaction picture.[4] The *time-ordering map* takes this string into $\mathcal{T}\{\tilde{q}_1(t_1)\cdots\tilde{q}_n(t_n)\} \equiv \varepsilon_\pi\,\tilde{q}_{\pi(1)}(t_{\pi(1)})\cdots\tilde{q}_{\pi(n)}(t_{\pi(n)})$, where $\pi \in \mathrm{S}_n$ is a permutation that puts the time arguments in chronological order, $t_{\pi(1)} > \cdots > t_{\pi(n)}$.

Notation A.1. Let us define the following notation for multivariate integrals by analogy with multi-index summations.[5]

$$\int_{t_1t_2t_3\ldots}^{[t_0,t]}dt_1dt_2dt_3\cdots \equiv \int_{t_0}^{t}dt_1\int_{t_0}^{t}dt_2\int_{t_0}^{t}dt_3\cdots \qquad \int_{t_1>t_2>t_3>\cdots}^{[t_0,t]}dt_1dt_2dt_3\cdots \equiv \int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\int_{t_0}^{t_2}dt_3\cdots \tag{A.5}$$

This notation should elucidate the following identity, which breaks an unrestricted integral into all possible chronologies.[6][7]

$$\int_{t_1\cdots t_n}^{[t_0,t]}dt_1\cdots t_n\,f(t_1\cdots t_n) = \sum_{\pi}^{\mathrm{S}_n}\int_{t_{\pi(1)}>\ldots>t_{\pi(n)}}^{[t_0,t]}dt_1\cdots t_n\,f(t_1\cdots t_n) \tag{A.6}$$

Proposition A.1. ***The Dyson series.*** *If $\tilde{V}(t)$ is particle-number consering, then $\tilde{U}(t,t_0) = \mathcal{T}\{e^{-i\int_{t_0}^{t}dt'\,\tilde{V}(t')}\}$.*

Proof: Expanding the time-ordered exponential in a Taylor series and applying equation A.6 gives the following

$$\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{t_1\cdots t_n}^{[t_0,t]}dt_1\cdots dt_n\,\mathcal{T}\{\tilde{V}(t_1)\cdots\tilde{V}(t_n)\} = \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\sum_{\pi}^{\mathrm{S}_n}\int_{t_{\pi(1)}>\ldots>t_{\pi(n)}}^{[t_0,t]}dt_1\cdots dt_n\,\mathcal{T}\{\tilde{V}(t_1)\cdots\tilde{V}(t_n)\} \tag{A.7}$$

which simplifies to equation A.4 because all $n!$ terms in the sum over chronologies are equal by def A.3.

Remark A.1. Assuming the boundary conditions of eq 9.4, the Dyson series for the wavefunction is

$$\tilde{\Psi}(t) = \lim_{t_0\to-\infty}\tilde{U}(t,t_0)\Psi(t_0) = \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{\mathbb{R}^n}dt_1\cdots dt_n\,\theta(t-t_1)\cdots\theta(t-t_n)\,\mathcal{T}\{\tilde{V}(t_1)\cdots\tilde{V}(t_n)\}\Psi_0 \tag{A.8}$$

where $\theta(x) = \int_{-\infty}^{x}dx'\delta(x')$ is the Heaviside step function, which here enforces the upper limits of integration.

[4] As in $\tilde{q}(t) \equiv e^{+iHt}qe^{-iHt}$ for some $q \in \{a_p\} \cup \{a_p^\dagger\}$.

[5] Compare these integrals to $\sum_{i_1i_2i_3\cdots}^{\{n_0,\ldots,n\}}$ and $\sum_{i_1>i_2>i_3\cdots}^{\{n_0,\ldots,n\}}$. The subscript defines the summation variables, along with any conditions restricting their values, and the superscript indicates the allowed range of values for each variable.

[7] The corresponding summation identity would be $\sum_{i_1\neq i_2\neq i_3\neq\cdots}^{\{n_0,n\}} = \sum_{\pi}^{\mathrm{S}_n}\sum_{i_{\pi(1)}>i_{\pi(2)}>i_{\pi(3)}>\cdots}^{\{n_0,n\}}$. The unrestricted integral is equivalent to an integral over $t_1 \neq t_2 \neq t_3 \neq \cdots$ because individual integrand values have "measure zero": $\int_{t_j}^{t_j}dt_i = 0$.

B Response functions

Definition B.1. ***Response functions.*** Any quantity $X(t)$ which depends on the time-envelopes $\{f_\beta(t)\}$ can be expanded in a Taylor series. The expansion coefficients in this series are called the *response functions* of $X(t)$.

$$X(t) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\beta_1,\dots,\beta_n} \int_{\mathbb{R}^n} dt_1 \cdots t_n \, f_{\beta_1}(t_1) \cdots f_{\beta_n}(t_n) \, X^{\beta_1 \cdots \beta_n}_{t;t_1 \cdots t_n} \qquad X^{\beta_1 \cdots \beta_n}_{t;t_1 \cdots t_n} \equiv \left. \frac{d^n X(t)}{df_{\beta_1}(t_1) \cdots df_{\beta_n}(t_n)} \right|_{\boldsymbol{f}=\mathbf{0}} \tag{B.1}$$

Example B.1. Substituting equation 9.2 into equation A.8 and comparing the result to equation B.1 implies the following.

$$\tilde{\Psi}^{\beta_1 \cdots \beta_n}_{t;t_1 \cdots t_n} = (-i)^n \theta(t - t_1) \cdots \theta(t - t_n) \, \mathcal{T}\{\tilde{V}_{\beta_1}(t_1) \cdots \tilde{V}_{\beta_n}(t_n)\} \Psi_0 \tag{B.2}$$

Defining $\tau_i \equiv t_i - t$, we find that wavefunction responses transform as follows when we move the time origin to t.[8]

$$\tilde{\Psi}^{\beta_1 \cdots \beta_n}_{0;\tau_1 \cdots \tau_n} = e^{-i(H - E_0)t} \, \tilde{\Psi}^{\beta_1 \cdots \beta_n}_{t;t_1 \cdots t_n} \tag{B.3}$$

Definition B.2. ***Property response functions.*** Response functions for the expectation value of an observable property W are usually denoted with the following double-brackets notation.

$$\langle\langle \tilde{W}(t); \tilde{V}_{\beta_1}(t_1), \dots, \tilde{V}_{\beta_n}(t_n) \rangle\rangle \equiv \left. \frac{d^n \langle \Psi(t) | W | \Psi(t) \rangle}{df_{\beta_1}(t_1) \cdots df_{\beta_n}(t_n)} \right|_{\boldsymbol{f}=\mathbf{0}} \tag{B.4}$$

In some contexts, these *property response functions* are known as *retarded propagators* or *retarded Green's functions*.

Example B.2. Substituting the response-function expansion of the wavefunction into $\langle \Psi(t) | W | \Psi(t) \rangle = \langle \tilde{\Psi}(t) | \tilde{W}(t) | \tilde{\Psi}(t) \rangle$ and grouping powers of $\boldsymbol{f}$ gives the following expression for property response functions.

$$\langle\langle \tilde{W}(t); \tilde{V}_{\beta_1}(t_1), \dots, \tilde{V}_{\beta_n}(t_n) \rangle\rangle = \sum_{p=0}^{n} \frac{1}{p!(n-p)!} \sum_{\pi}^{\mathrm{S}_n} \langle \tilde{\Psi}^{\beta_{\pi(1)} \cdots \beta_{\pi(p)}}_{t;t_{\pi(1)} \cdots t_{\pi(p)}} | \tilde{W}(t) | \tilde{\Psi}^{\beta_{\pi(p+1)} \cdots \beta_{\pi(n)}}_{t;t_{\pi(p+1)} \cdots t_{\pi(n)}} \rangle \tag{B.5}$$

Using equation B.3 and $\tilde{W}(t) = e^{-iHt} \tilde{W}(0) e^{+iHt}$, we can show that the property responses are invariant to time translation.

$$\langle\langle \tilde{W}(0); \tilde{V}_{\beta_1}(\tau_1), \dots, \tilde{V}_{\beta_n}(\tau_n) \rangle\rangle = \langle\langle \tilde{W}(t); \tilde{V}_{\beta_1}(t_1), \dots, \tilde{V}_{\beta_n}(t_n) \rangle\rangle \tag{B.6}$$

Proposition B.1. ***Linear property response function.*** $\langle\langle \tilde{W}(t); \tilde{V}_\beta(t') \rangle\rangle = -i\theta(t - t') \langle \Psi_0 | [\tilde{W}(t), \tilde{V}_\beta(t')] | \Psi_0 \rangle$

Proof: This follows from equations B.2 and B.5 with $n = 1$.

Corollary B.1. *Defining $\omega_k \equiv E_k - E_0$ and $\tau \equiv t' - t$, the linear property reponse can be expressed as follows.*

$$\langle\langle \tilde{W}(t); \tilde{V}_\beta(t') \rangle\rangle = -i\theta(-\tau) \sum_{k=0}^{\infty} (e^{+i\omega_k \tau} \langle \Psi_0 | W | \Psi_k \rangle \langle \Psi_k | V_\beta | \Psi_0 \rangle - e^{-i\omega_k \tau} \langle \Psi_0 | V_\beta | \Psi_k \rangle \langle \Psi_k | W | \Psi_0 \rangle)$$

Proof: Expanding the interaction-picture operators of prop B.1 in the Schrödinger picture yields the following

$$\langle\langle \tilde{W}(t); \tilde{V}_\beta(t') \rangle\rangle = -i\theta(t - t')(\langle \Psi_0 | W e^{-i(H - E_0)(t - t')} V_\beta | \Psi_0 \rangle - \langle \Psi_0 | V_\beta e^{-i(H - E_0)(t' - t)} W | \Psi_0 \rangle) \tag{B.7}$$

since $H\Psi_0 = E_0 \Psi_0$. The proposition follows from a spectral resolution of $e^{\mp(H - E_0)(t - t')}$ in each term.

Definition B.3. ***Response functions (frequency domain).*** The frequency-domain response functions of $X(t)$ at $t = 0$ are defined as ϵ-shifted Fourier transforms of the time-domain response functions with respect to $\tau_1, \dots, \tau_n$.

$$X^{\beta_1 \cdots \beta_n}_{0;\tau_1 \cdots \tau_n} = (2\pi)^{-n} \int_{\mathbb{R}^n} d\omega_1 \cdots d\omega_n \, X^{\beta_1 \cdots \beta_n}_{\omega_{\epsilon,1} \cdots \omega_{\epsilon,n}} e^{+i \sum_j \omega_{\epsilon,j} \tau_j} \qquad X^{\beta_1 \cdots \beta_n}_{\omega_{\epsilon,1} \cdots \omega_{\epsilon,n}} \equiv \int_{\mathbb{R}^n} d\tau_1 \cdots d\tau_n \, X^{\beta_1 \cdots \beta_n}_{0;\tau_1 \cdots \tau_n} e^{-i \sum_j \omega_{\epsilon,j} \tau_j} \tag{B.8}$$

From equations 9.5 and B.1, we find that these are coefficients in the frequency-envelope Taylor expansion of $X(0)$.

$$X(0) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\beta_1 \cdots \beta_n} \int_{\mathbb{R}^n} d\omega_1 \cdots d\omega_n \, f_{\beta_1}(\omega_{\epsilon,1}) \cdots f_{\beta_n}(\omega_{\epsilon,n}) \, X^{\beta_1 \cdots \beta_n}_{\omega_{\epsilon,1} \cdots \omega_{\epsilon,n}} \qquad X^{\beta_1 \cdots \beta_n}_{\omega_{\epsilon,1} \cdots \omega_{\epsilon,n}} = \left. \frac{d^n X(0)}{df_{\beta_1}(\omega_{\epsilon,1}) \cdots df_{\beta_n}(\omega_{\epsilon,n})} \right|_{\boldsymbol{f}=\mathbf{0}} \tag{B.9}$$

Property response functions in the frequency domain are denoted by $\langle\langle W; V_{\beta_1}, \dots, V_{\beta_n} \rangle\rangle_{\omega_{\epsilon,1} \cdots \omega_{\epsilon,n}}$, which can be written as a Fourier transform of $\langle\langle \tilde{W}(t); \tilde{V}_{\beta_1}(t_1), \dots, \tilde{V}_{\beta_n}(t_n) \rangle\rangle$ itself due to its translational invariance. Prop B.2 shows that these frequency-domain functions can be used to expand $\langle \Psi(t) | W | \Psi(t) \rangle$ away from the time origin.

[8] This follows from $\theta(t - t_i) = \theta(0 - \tau_i)$ and $\tilde{V}_{\beta_i}(\tau_i) = e^{-iHt} \tilde{V}_{\beta_i}(t_i) e^{+iHt} \implies \tilde{V}_{\beta_1}(\tau_1) \cdots \tilde{V}_{\beta_n}(\tau_n) = e^{-iHt} \tilde{V}_{\beta_1}(t_1) \cdots \tilde{V}_{\beta_n}(t_n) e^{+iHt}$.

Proposition B.2. *The expectation value of an observable W at time t is given by the following.*

$$\langle\Psi(t)|W|\Psi(t)\rangle = \sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\beta_1,\ldots,\beta_n}\int_{\mathbb{R}^n} d\omega_1\cdots d\omega_n\, f_{\beta_1}(\omega_{\epsilon,1})\cdots f_{\beta_n}(\omega_{\epsilon,n})\,\langle\langle W; V_{\beta_1},\ldots,V_{\beta_n}\rangle\rangle_{\omega_{\epsilon,1}\cdots\omega_{\epsilon,n}}\, e^{-i\sum_j \omega_{\epsilon,j} t}$$

Proof: This follows from substituting equation 9.5 into the time-envelope expansion and inserting $e^{-i\sum_j \omega_{\epsilon,j}t}e^{+i\sum_j \omega_{\epsilon,j}t}$.

Remark B.1.

$$\langle\langle \tilde{W}(t); \tilde{V}_\beta(t')\rangle\rangle = \sum_{k=0}^{\infty}(g_k^+(\tau)\langle\Psi_0|W|\Psi_k\rangle\langle\Psi_k|V_\beta|\Psi_0\rangle - g_k^-(\tau)\langle\Psi_0|V_\beta|\Psi_k\rangle\langle\Psi_k|W|\Psi_0\rangle) \quad g_k^{\pm}(\tau)\equiv -i\theta(-\tau)e^{\pm i\omega_k\tau} \tag{B.10}$$

$$g_k^{\pm}(\omega_\epsilon) = \int_{-\infty}^{\infty} d\tau\, g_k^{\pm}(\tau)e^{-i\omega_\epsilon\tau} = -i\int_{-\infty}^{0} d\tau\, e^{-i(\omega_\epsilon\mp\omega_k)\tau} = \frac{1}{\omega_\epsilon\mp\omega_k} \tag{B.11}$$

$$g_k^{\pm}(\tau) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, g_k^{\pm}(\omega_\epsilon)e^{+i\omega_\epsilon\tau} = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \frac{e^{+i\omega_\epsilon\tau}}{\omega_\epsilon\mp\omega_k} \tag{B.12}$$

C Complex analysis

Definition C.1. ***Continuity.*** A complex-valued function f is said to be *continuous* at $z \in \mathbb{C}$ if for any positive real number ϵ we can choose a radius $\delta > 0$ such that all complex values z' within δ of z satisfy $|f(z') - f(z)| < \epsilon$. That is, we can always choose a circle small enough that all function values lie within some threshold.

Definition C.2. ***Holomorphic function.*** The function $f(z)$ is *differentiable* at z if the following limit exists and has the same value with h approaching from any direction in the complex plane.

$$\frac{\partial f(z)}{\partial z} \equiv \lim_{h\to 0} \frac{f(z+h) - f(z)}{h} \tag{C.1}$$

A *holomorphic function* is a complex-valued function which is differentiable everywhere on $\mathbb{C}$.

Definition C.3. ***Wirtinger derivatives.*** Denoting the real and imaginary components of z by x and y we find

$$z = x + iy \qquad \Longrightarrow \qquad dz = dx + idy, \quad dz^* = dx - idy \qquad \Longrightarrow \qquad dx = \tfrac{1}{2}\left(dz + dz^*\right), \quad dy = \tfrac{1}{2i}\left(dz - dz^*\right) \tag{C.2}$$

by adding and subtracting differentials. Comparing these to the total derivative expansion for each variable, we find

$$\frac{\partial x}{\partial z} = \frac{1}{2} \qquad \frac{\partial x}{\partial z^*} = \frac{1}{2} \qquad \frac{\partial y}{\partial z} = \frac{1}{2i} \qquad \frac{\partial y}{\partial z^*} = -\frac{1}{2i} \tag{C.3}$$

which can lead to the following formulas for derivatives with respect to z and z^*, known as *Wirtinger derivatives*.

$$\frac{\partial}{\partial z} = \frac{\partial x}{\partial z}\frac{\partial}{\partial x} + \frac{\partial y}{\partial z}\frac{\partial}{\partial y} = \frac{1}{2}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right) \qquad \frac{\partial}{\partial z^*} = \frac{\partial x}{\partial z^*}\frac{\partial}{\partial x} + \frac{\partial y}{\partial z^*}\frac{\partial}{\partial y} = \frac{1}{2}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right) \tag{C.4}$$

These can be used to show that $\frac{\partial z^*}{\partial z} = \frac{\partial z}{\partial z^*} = 0$, confirming that z and z^* are independent variables.

Proposition C.1. *The function f is differentiable at z if and only if* $\dfrac{\partial f(z)}{\partial z^*} = 0$.

Proof: Let $z = x + iy$ and assume the derivatives with respect to x and y exist. Then we can express $f(z+h) - f(h)$ as a bivariate Taylor expansion in $\mathrm{Re}(h)$ and $\mathrm{Im}(h)$, whose linear term is given by the following.

$$\frac{\partial f(z)}{\partial x}\mathrm{Re}(h) + \frac{\partial f(z)}{\partial y}\mathrm{Im}(h) = \frac{\partial f(z)}{\partial x}\frac{h + h^*}{2} + \frac{\partial f(z)}{\partial y}\frac{h - h^*}{2i}$$

Dividing this expression by h and taking the limit as $h \to 0$ gives the complex derivative of f at z.

$$\lim_{h\to 0}\frac{f(z+h) - f(z)}{h} = \frac{1}{2}\left(\frac{\partial f(z)}{\partial x} + \frac{1}{i}\frac{\partial f(z)}{\partial y}\right) + \frac{1}{2}\left(\frac{\partial f(z)}{\partial x} - \frac{1}{i}\frac{\partial f(z)}{\partial y}\right)\lim_{h\to h^*}\frac{h^*}{h}$$

If h approaches along the real axis, the limit of h^*/h is $+1$. If h approaches along the imaginary axis, the limit of h^*/h is -1. Therefore, f is differentiable if and only if $\frac{1}{2}\left(\frac{\partial f(z)}{\partial x} - \frac{1}{i}\frac{\partial f(z)}{\partial y}\right) = 0$, which is equivalent to $\frac{\partial f(z)}{\partial z^*} = 0$. If the derivatives with respect to x and y do not exist then f is not differentiable and $\frac{\partial f(z)}{\partial z^*}$ is undefined.

Notation C.1. ***Complex integration.*** The notation $\int_\gamma dz\, f(z)$ denotes the line integral of f over a path γ in the complex plane, which is known as *contour integration*. The notation $\oint_\gamma dz\, f(z)$ means that γ is a closed and counterclockwise.

Proposition C.2. *If γ is a circular path containing the point z, then* $\displaystyle\oint_\gamma dz'\, \frac{1}{z' - z} = 2\pi i$.

Proof: We can assume without loss of generality that z is at the origin and parametrize the path as $z'(\theta) = re^{i\theta}$. Given that $dz'(\theta) = ire^{i\theta}d\theta$, we have $dz'(\theta)\, z'(\theta)^{-1} = id\theta$. Integrating from 0 to 2π concludes the proof.

D The generalized Stokes' theorem

Definition D.1. ***Topological space.*** Let X be a set and let T_X be a family of subsets of X. T_X qualifies as a *topology* if

1. T_X contains the empty set and X itself. $\emptyset \in T_X,\ X \in T_X.$
2. Any finite or infinite union of sets in T_X is in T_X. $\{O_i \,|\, i \in I\} \subseteq T_X \implies \cup_{i\in I} O_i \in T_X$
3. Any finite intersection of sets in T_X is in T_X. $\{O_i \,|\, 1 \leq i \leq n\} \subseteq T_X \implies \cap_{i=1}^{n} O_i \in T_X$

in which case we call (X, T_X) a *topological space*. The elements of X are called *points* and the elements of T_X are called *open subsets*. For an arbitrary subset V of X, not necessarily open, we say that V is a *neighborhood* of the point $x \in X$ if it contains an open set O containing x.[9]

Definition D.2. ***Homeomorphism.*** A function $f : X \to X'$ between topological spaces (X, T_X) and $(X', T_{X'})$ is said to be *surjective* if it maps onto all of X'.[10] This function is *continuous* if the preimage of any open subset in T_X is an open subset in $T_{X'}$.[11] If it has a continuous inverse, we say that f is *bicontinuous*. A surjective, bicontinuous function is called a *homeomorphism*. If there is a homeomorphism between two topological spaces, we call them *homeomorphic*.

Theorem D.1. *.*

[9] That is, if $x \in O \subseteq V$.

[10] In other words every $x' \in X$ can be written as $x' = f(x)$ for some $x \in X$.

[11] The preimage image of the open set $O' \in T_{X'}$ is $f^{-1}(O') = \{x \in X \,|\, f(x) \in O'\}$.