9 Response theory

A Time-dependent perturbation theory

Remark A.1. In an time-varying field, the electronic wavefunction is no longer simply an eigenfunction of the Hamiltonian. This more general system is described by the following *time-dependent Schrödinger equation*

$$H(t)\Psi(t) = i\frac{\partial\Psi(t)}{\partial t} \qquad\qquad H(t) = H + V(t) \tag{A.1}$$

where H is the usual electronic Hamiltonian and $V(t)$ describes the interaction with the external field. If the electrons are prepared in a particular state Ψ_0 at some time t_0, the system is completely described by a *time-evolution operator*.

$$\Psi(t) = U(t, t_0)\Psi_0 \qquad\qquad \Psi_0 = \Psi(t_0) \tag{A.2}$$

The following discussion shows how to expand this operator in orders of the perturbing interaction, $V(t)$.

Definition A.1. ***Interaction picture.*** The *interaction picture* results from to the following similarity transformation.

$$\tilde{\Theta}(t) \equiv e^{+iHt}\Theta(t) \qquad\qquad \tilde{W}(t) \equiv e^{+iHt}W(t)e^{-iHt} \tag{A.3}$$

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

$$\tilde{V}(t)\tilde{\Psi}(t) = i\frac{\partial\tilde{\Psi}(t)}{\partial t} \tag{A.4}$$

Multiplying both sides by $-i$ and integrating from t_0 to t yields a recursive equation for the interaction-picture wavefunction

$$\tilde{\Psi}(t) - \tilde{\Psi}(t_0) = -i\int_{t_0}^{t} dt'\,\tilde{V}(t')\tilde{\Psi}(t') \tag{A.5}$$

from which we infer $\tilde{U}(t, t_0) = 1 - i\int_{t_0}^{t} dt'\tilde{V}(t')\,\tilde{U}(t', t_0)$. Infinite recursion of this identity leads to the following.

$$\tilde{U}(t, t_0) = \sum_{n=0}^{\infty}(-i)^n\int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2\cdots\int_{t_0}^{t_{n-1}} dt_n\,\tilde{V}(t_1)\cdots\tilde{V}(t_n) \tag{A.6}$$

Definition A.2. ***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.[1] 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 reverse-chronological order, $t_{\pi(1)} > \cdots > t_{\pi(n)}$.

Notation A.1.

$$\int_{t_1,t_2,t_3,\dots}^{[t_0,t]} dt_1dt_2dt_3\cdots \equiv \int_{t_0}^{t} dt_1\int_{t_0}^{t} dt_2\int_{t_0}^{t} dt_3\cdots \qquad \int_{t_1>t_2>t_3>\cdots}^{[t_0,t]} dt_1dt_2dt_3\cdots \equiv \int_{t_0}^{t} dt_1\int_{t_0}^{t_1} dt_2\int_{t_0}^{t_2} dt_3\cdots \tag{A.7}$$

$$\int_{t_1\cdots t_n}^{[t_0,t]} dt_1\cdots t_n\,f(t_1\cdots t_n) = \sum_{\pi\in\mathrm{S}_n}\int_{t_{\pi(1)}>\dots>t_{\pi(n)}}^{[t_0,t]} dt_1\cdots t_n\,f(t_1\cdots t_n) \tag{A.8}$$

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

Proof:

$$\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{t_1\cdots t_n}^{[t_0,t]} dt_1\cdots dt_n\,\mathcal{T}\{\tilde{V}(t_1)\cdots\tilde{V}(t_n)\} = \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\sum_{\pi\in\mathrm{S}_n}\int_{t_{\pi(1)}>\dots>t_{\pi(n)}}^{[t_0,t]} dt_1\cdots dt_n\,\mathcal{T}\{\tilde{V}(t_1)\cdots\tilde{V}(t_n)\} \tag{A.9}$$

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

B Response functions

Remark B.1.

$$V(t) = \sum_{\beta} V_\beta f_\beta(t) \qquad \lim_{t\to-\infty} f_\beta(t) = 0 \tag{B.1}$$

$$\tilde{\Psi}^{(0)}(t) = \lim_{t\to-\infty} \tilde{\Psi}(t) = \Psi_0 \qquad H\Psi_k = E_k\Psi_k \tag{B.2}$$

$$\tilde{\Psi}(t) = \sum_{n=0}^{\infty} \tilde{\Psi}^{(n)}(t) \qquad \tilde{\Psi}^{(n)}(t) = \frac{(-i)^n}{n!}\int_{\mathbb{R}^n} dt_1\cdots dt_n\,\theta(t-t_1)\cdots\theta(t-t_n)\,\mathcal{T}\{\tilde{V}(t_1)\cdots\tilde{V}(t_n)\}\Psi_0 \tag{B.3}$$

Definition B.1. ***Response function.***

$$X(t) = \sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\beta_1,\dots,\beta_n}\int_{\mathbb{R}^n} dt_1\cdots t_n\, f_{\beta_1}(t_1)\cdots f_{\beta_n}(t_n)\, X^{\beta_1\cdots\beta_n}_{t;t_1\cdots t_n} \qquad X^{\beta_1\cdots\beta_n}_{t;t_1\cdots t_n} \equiv \left.\frac{d^nX(t)}{df_{\beta_1}(t_1)\cdots df_{\beta_n}(t_n)}\right|_{\boldsymbol{f}=\boldsymbol{0}} \tag{B.4}$$

Proposition B.1.

$$\Psi^{\beta_1\cdots\beta_n}_{t;t_1\cdots t_n} = (-i)^n\theta(t-t_1)\cdots\theta(t-t_n)\,\mathcal{T}\{\tilde{V}(t_1)\cdots\tilde{V}(t_n)\}\Psi_0 \tag{B.5}$$

Notation B.1.

$$\langle\langle\tilde{W}(t);\tilde{V}_{\beta_1}(t_1),\dots,\tilde{V}_{\beta_n}(t_n)\rangle\rangle \equiv \left.\frac{d^n\langle\Psi(t)|W(t)|\Psi(t)\rangle}{df_{\beta_1}(t_1)\cdots df_{\beta_n}(t_n)}\right|_{\boldsymbol{f}=\boldsymbol{0}} \tag{B.6}$$

Example B.1.

$$\tilde{\Psi}^{\beta}_{t;t'} = \left.\frac{\partial\tilde{\Psi}(t)}{\partial f_\beta(t')}\right|_{\boldsymbol{f}=\boldsymbol{0}} = \tag{B.7}$$

C Fourier transforms

Remark C.1.

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

$f_\beta(-\omega) = f_\beta^*(\omega)$

Footnote: Fourier transforms can always be verified using $\int_{\mathbb{R}} dk\, e^{ikx} = 2\pi\, \delta(x)$

Remark C.2. Define $\tau_j \equiv t_j - t$ and note that $X^{\beta_1\cdots\beta_n}_{t;t_1\cdots t_n} = X^{\beta_1\cdots\beta_n}_{0;\tau_1\cdots\tau_n}$

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

Remark C.3. $\int_{\mathbb{R}^n} dt_1 \cdots dt_n\, f_{\beta_1}(t_1) \cdots f_{\beta_n}(t_n)\, X^{\beta_1\cdots\beta_n}_{t;t_1\cdots t_n} = \int_{\mathbb{R}^n} d\omega_1 \cdots d\omega_n\, f_{\beta_1}(\omega_1) \cdots f_{\beta_n}(\omega_n) X^{\beta_1\cdots\beta_n}_{\omega_1\cdots\omega_n} e^{-i\sum_j \omega_j t}$

D Complex Calculus