Magnus Expansion

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Statement: Consider a Bloch Hamiltonian with periodic monochromatic perturbation $H(t)$: For time $t > T(\equiv 2\pi/\omega_0)$, the effective Hamiltonian describing the system is

$$H_{eff} = H_0 + \frac{[H_{-1}, H_1]}{\omega_0} + \mathcal{O}\left(\frac{1}{\omega_0^2}\right) \tag{1}$$

where

$$H(t) = \sum_m H_m \exp(im\omega_0 t) \qquad H_m = \frac{1}{T}\int_0^T dt H(t) \exp(-im\omega_0 t) \tag{2}$$

Proof:
The time-evolution operator satisfies

$$\begin{aligned} & i\hbar\frac{\partial}{\partial t}U(t,t_0) = \lambda H(t)U(t,t_0) \\ & \Rightarrow U(t,t_0) = \hat{T}_t \exp\left(-\frac{i}{\hbar}\lambda\int_{t_0}^{t} dt' H(t')\right) \equiv \exp\left[\Omega(t,t_0)\right] \quad : \text{Magnus Solution} \end{aligned} \tag{3}$$

λ here is kept for book-keeping purposes useful when expanding the exponent. Defining an anti-Hermitian Hamiltonian

$$\tilde{H}(t) = -\frac{i}{\hbar}H(t) \qquad \tilde{H}(t)^\dagger = -\tilde{H}(t) \tag{4}$$

To proceed further, we will need Baker-Campbell-Hausdorff (BCH) formula

$$\exp(x)\exp(y) = \exp\left(x + y + \frac{1}{2}[x,y] + \frac{1}{12}[x,[x,y]] + ...\right) \tag{5}$$

where x and y are non-commutative operators. Thus we can collect terms upto first order in x in the above expansion

$$\exp(x)\exp(y) = \exp\left(x + y + \sum_{k=1}^{\infty}(-1)^k \frac{B_k}{k!}[y,[...,[y,x]]]\Big|_{k-\text{times}} + \mathcal{O}(x^2)\right) \tag{6}$$

where

$$[y,[...,[y,x]]]\Big|_{k-\text{times}} = \begin{cases} [y,x] & k=1 \\ [y,[y,x]] & k=2 \\ [y,[y,[y,x]]] & k=3 \\ ... \\ ... \\ ... \end{cases}$$

The time-evolution operator has the property

$$U(t+\delta t, t_0) = U(t+\delta t, t)U(t,t_0) = \exp\left(\lambda\tilde{H}(t)\delta t\right)U(t,t_0) \tag{7}$$

given δt is infinitesimally small time increment. By the definition of Magnus Solution

$$U(t+\delta t, t_0) = \exp\left[\Omega(t+\delta t, t_0)\right] \tag{8}$$

Using the BCH formula for terms upto linear order in δt

$$\exp\left(\lambda\tilde{H}(t)\delta t\right)U(t,t_0) = \exp\left(\Omega(t,t_0) + \lambda\tilde{H}(t)\delta t + \sum_{k=1}^{\infty}(-1)^k\frac{B_k}{k\,!}\left[\Omega(t,t_0),\left[...,[\Omega(t,t_0),\lambda\tilde{H}(t)\delta t]\right]\right]\Big|_{k-\text{times}}\right) \tag{9}$$

Thus upon comparison $U(t+\delta t,t_0) = U(t+\delta t,t)U(t,t_0)$

$$\Omega(t+\delta t,t_0) = \Omega(t,t_0) + \lambda\delta t\left[\tilde{H}(t) + \sum_{k=1}^{\infty}(-1)^k\frac{B_k}{k\,!}\left[\Omega(t,t_0),\left[...,[\Omega(t,t_0),\tilde{H}(t)]\right]\right]\Big|_{k-\text{times}}\right] \tag{10}$$

which leads to a differential equation in $\Omega(t,t_0)$

$$\frac{\partial}{\partial t}\Omega(t,t_0) = \lambda\tilde{H}(t) + \lambda\sum_{k=1}^{\infty}(-1)^k\frac{B_k}{k\,!}\left[\Omega(t,t_0),\left[...,[\Omega(t,t_0),\tilde{H}(t)]\right]\right]\Big|_{k-\text{times}} \tag{11}$$

Magnus proposed that the exponent can be expanded in a series in parameter λ

$$\Omega(t,t_0) = \sum_{k=1}^{\infty}\lambda^k\Omega_k(t,t_0) = \lambda^1\Omega_1(t,t_0) + \lambda^2\Omega_2(t,t_0) + ... \tag{12}$$

Substituting this series expansion in the differential equation for $\Omega(t,t_0)$ and comparing terms order by order (in λ):

$$\frac{\partial}{\partial t}\Omega_1(t,t_0) = \tilde{H}(t) \Rightarrow \Omega_1(t,t_0) = \int_{t_0}^{t}dt'\,\tilde{H}(t') \tag{13}$$

$$\begin{aligned}\frac{\partial}{\partial t}\Omega_2(t,t_0) = -\frac{1}{2}[\Omega_1(t,t_0),\tilde{H}(t)] \Rightarrow \Omega_2(t,t_0) &= -\frac{1}{2}\int_{t_0}^{t}dt'\,[\Omega_1(t',t_0),\tilde{H}(t')]\\ &= \frac{1}{2}\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\,[\tilde{H}(t_1),\tilde{H}(t_2)]\end{aligned} \tag{14}$$

Therefore

$$U(t,t_0) = \exp\left(\Omega(t,t_0)\right) \equiv \hat{T}_t\exp\left(\lambda\int_{t_0}^{t}dt'\,\tilde{H}(t')\right) \tag{15}$$

$$U(T,0) = \exp\left(\Omega(T,0)\right)|_{\lambda=1} \equiv \exp\left(-\frac{i}{\hbar}H_{eff}T\right) \tag{16}$$

Thus we can read the effective Hamiltonian

$$H_{eff} = \frac{1}{T}\int_0^T dt\,H(t) - \frac{i}{\hbar}\frac{1}{2T}\int_0^T dt_1\int_0^{t_1}dt_2\,[H(t_1),H(t_2)] \tag{17}$$

Using

$$H(t) = \sum_m H_m\exp\left(im\omega_0 t\right) \quad H_m = \frac{1}{T}\int_0^T dtH(t)\exp\left(-im\omega_0 t\right) \tag{18}$$

$$H_0 = \frac{1}{T}\int_0^T dtH(t) \tag{19}$$

$$\frac{1}{2T}\int_0^T dt_1\int_0^{t_1}dt_2\,[H(t_1),H(t_2)] = \sum_{n=1}^{\infty}\frac{1}{in\omega_0}\left([H_{-n},H_n] - \frac{1}{2}[H_0,H_n] + \frac{1}{2}[H_0,H_{-n}]\right) \tag{20}$$

Hence upto first order

$$H_{eff} = H_0 - \frac{i}{\hbar}\sum_{n=1}^{\infty}\frac{1}{in\omega_0}\left([H_{-n},H_n] - \frac{1}{2}[H_0,H_n] + \frac{1}{2}[H_0,H_{-n}]\right) \tag{21}$$

The maximum contribution comes from $n = 1$

$$H_{eff} = H_0 - \frac{1}{\hbar\omega_0}\left([H_{-1},H_1] - \frac{1}{2}[H_0,H_1] + \frac{1}{2}[H_0,H_{-1}]\right) \tag{22}$$