Adiabatic Conditions of Time-dependent Rice-Mele model

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I. ADIABATIC CONDITIONS GENERAL

Suppose we have some time-dependent Hamiltonian $H(t)$. For arbitrary time t, there are instant eigenstates corresponding to instant eigenvalues of $H(t)$

$$H(t)|n(t)\rangle = E_n(t)|n(t)\rangle \tag{1}$$

which constitutes a set of complete bases for the system. Any state $|psi(t)\rangle$ could be expanded as

$$|\psi(t)\rangle = \sum_n a_n(t)e^{\mathrm{i}\theta_n(t)}|n(t)\rangle \tag{2}$$

Here $\theta_n(t) = (-1/\hbar)\int^t dt' E_n(t')$. Now we have not specified the phase choosing for $|n(t)\rangle$. But this should not affect the adiabatic approximation as well as Berry phase. Consider some state $|\psi(t)\rangle$ satisfies time-dependent Schrödinger equation

$$\mathrm{i}\hbar\partial_t|\psi(t)\rangle = H(t)|\psi(t)\rangle \tag{3}$$

Substitute Eq (2) into it yields

$$\begin{aligned}
\text{left} =&\mathrm{i}\hbar\sum_n[(\dot{a}_n(t) + a_n(t)\mathrm{i}\partial_t\theta_n(t))e^{\mathrm{i}\theta_n(t)} + a_n(t)e^{\mathrm{i}\theta_n(t)}\partial_t]|n(t)\rangle \\
=&\mathrm{i}\hbar\sum_n \dot{a}_n(t)e^{\mathrm{i}\theta_n(t)}|n(t)\rangle \\
&+\sum_n E_n(t)a_n(t)e^{\mathrm{i}\theta_n(t)}|n(t)\rangle \\
&+\mathrm{i}\hbar\sum_n a_n(t)e^{\mathrm{i}\theta_n(t)}\partial_t|n(t)\rangle \\
\text{right} =&\sum_n E_n(t)a_n(t)e^{\mathrm{i}\theta_n(t)}|n(t)\rangle
\end{aligned}$$

Right side cancels the second term of left side, which results in

$$\sum_n \dot{a}_n(t)e^{\mathrm{i}\theta_n(t)}|n(t)\rangle + a_n(t)e^{\mathrm{i}\theta_n(t)}\partial_t|n(t)\rangle = 0$$

Act $\langle m(t)|$ from the left

$$\langle m(t)|\sum_n \dot{a}_n(t)e^{\mathrm{i}\theta_n(t)}|n(t)\rangle + a_n(t)e^{\mathrm{i}\theta_n(t)}\partial_t|n(t)\rangle = 0$$

$$\therefore \dot{a}_m(t) = -\sum_n a_n(t)e^{\mathrm{i}[\theta_n(t)-\theta_m(t)]}\langle m(t)|\partial_t n(t)\rangle$$

Notice that for $m \neq n$

$$\begin{aligned}\partial_t\langle m(t)|H(t)|n(t)\rangle &= \langle\partial_t m(t)|H(t)|n(t)\rangle + \langle m(t)|\partial_t H(t)|n(t)\rangle + \langle m(t)|H(t)|\partial_t n(t)\rangle \\ &= -(E_n - E_m)\langle m(t)|\partial_t n(t)\rangle + \langle m(t)|\partial H/\partial t|n(t)\rangle\end{aligned}$$

we have

$$\langle m(t)|\partial_t n(t)\rangle = \frac{\langle m|\partial H/\partial t|n\rangle}{E_n - E_m}$$

Thus

$$\begin{aligned}\dot{a}_m(t) &= -\sum_n a_n(t)e^{\mathrm{i}[\theta_n(t)-\theta_m(t)]}\langle m(t)|\partial_t n(t)\rangle \\ &= -a_m(t)\langle m(t)|\partial_t m(t)\rangle - \sum_{n\neq m} a_n(t)e^{\mathrm{i}[\theta_n(t)-\theta_m(t)]}\frac{\langle m(t)|\partial H/\partial t|n(t)\rangle}{E_n(t) - E_m(t)}\end{aligned}$$

Suppose we start at the nth eigen state of the system, i.e.

$$\begin{aligned}&a_n(0) = 1 \\ &a_{n'\neq n}(0) = 0 \quad (\text{for } n \neq 0)\end{aligned}$$

Then to first order approximation,

$$\begin{aligned}\dot{a}_m(t) &= -a_n(t)\exp\left[-\frac{\mathrm{i}}{\hbar}\int^t E_n(t') - E_m(t')dt'\right]\langle m(t)|\partial_t n(t)\rangle \\ &= -a_n(t)\exp\left[-\frac{\mathrm{i}}{\hbar}\int^t E_n(t') - E_m(t')dt'\right]\frac{\langle m(t)|\partial H/\partial t|n(t)\rangle}{E_n(t) - E_m(t)}\end{aligned}$$

- Niu's:

$$a_m(t) = -\frac{\langle m|\partial_t|n\rangle}{E_n - E_m}\mathrm{i}\hbar\exp\left[-\frac{\mathrm{i}}{\hbar}\int^t E_n(t') - E_m(t')dt'\right]$$

adiabatic condition:

$$-\frac{\langle m|\partial_t|n\rangle}{E_n - E_m}\mathrm{i}\hbar \ll 1$$

- Sakurai's:

$$\frac{\langle m(t)|\partial H/\partial t|n(t)\rangle}{E_n(t)-E_m(t)} \equiv \frac{1}{\tau} \ll \langle m(t)|\partial_t m(t)\rangle \sim \frac{E_m}{\hbar}$$

II. TIME-DEPENDENT RM

Suppose time dependence

$$\begin{aligned}\delta(t) &= \delta\sin(\omega t)\\ \Delta(t) &= \Delta\cos(\omega t)\end{aligned}$$

then

$$H(t) = \sum_j -(J+\delta\sin(\omega t))a_j^\dagger b_j - (J-\delta\sin(\omega t))a_{j+1}^\dagger b_j + h.c. + \Delta\cos(\omega t)(a_j^\dagger a_j - b_j^\dagger b_j)$$

and $\mathcal{F}.\mathcal{T}$.

$$H = \sum_q \begin{pmatrix} a_q^\dagger & b_q^\dagger \end{pmatrix} \mathcal{H}(q) \begin{pmatrix} a_q \\ b_q \end{pmatrix}$$

where $\mathcal{H}(q) = \boldsymbol{h}(q)\cdot\boldsymbol{\sigma}$, and

$$\begin{aligned}\boldsymbol{h}(q,t) &= (-2J\cos(\frac{qa}{2}), -2\delta\sin(\omega t)\sin(\frac{qa}{2}), \Delta\cos(\omega t))\\ \boldsymbol{\sigma} &= (\sigma_x, \sigma_y, \sigma_z)\end{aligned}$$

Instant eigenenergies

$$\mathcal{E}_\pm(q,t) = \pm\sqrt{4J^2\cos^2(\frac{qa}{2}) + 4\delta^2\sin^2(\omega t)\sin^2(\frac{qa}{2}) + \Delta^2\cos^2(\omega t)}$$

and corresponding eigenstates

$$\begin{aligned}\psi_+(x;q,t) &= e^{\mathrm{i}qx}\begin{pmatrix}\cos\frac{\theta}{2}e^{-\mathrm{i}\phi}\\ \sin\frac{\theta}{2}\end{pmatrix}\\ \psi_-(x;q,t) &= e^{\mathrm{i}qx}\begin{pmatrix}\sin\frac{\theta}{2}e^{-\mathrm{i}\phi}\\ -\cos\frac{\theta}{2}\end{pmatrix}\end{aligned}$$

where θ, ϕ are as functions of q, t.

- Niu's:

$$
\begin{aligned}
E_+ - E_- &= 2|\boldsymbol{h}(q,t)| \\
\langle +;q,t|\partial_t|-;q,t\rangle &= (-\mathrm{i})\sin^2(\theta/2)\frac{d\phi}{dt} \\
\therefore -\frac{\langle +;q,t|\partial_t|-;q,t\rangle}{E_- - E_+}\mathrm{i}\hbar &= \frac{\hbar\sin^2(\theta/2)\frac{d\phi}{dt}}{2|\mathcal{E}(q,t)|} \ll 1
\end{aligned}
$$

approximately, this means $\hbar\omega \ll \text{Minimum}[J,\delta,\Delta]$.

- Sakurai's:

$$
\dot{\boldsymbol{h}}(q,t) = (0, -2\delta\omega\cos(\omega t)\sin(qa/2), -\Delta\omega\sin(\omega t))
$$

$$
\begin{aligned}
\langle +;q,t|\partial\mathcal{H}(q,t)/\partial t|-;q,t\rangle &= \langle +;q,t|\dot{\boldsymbol{h}}\cdot\boldsymbol{\sigma}|-;q,t\rangle \\
&= -2\delta\omega\cos(\omega t)\sin(qa/2)\langle +|\sigma_y|-\rangle - \Delta\omega\sin(\omega t)\langle +|\sigma_z|-\rangle
\end{aligned}
$$

While

$$
\begin{aligned}
\langle +|\sigma_y|-\rangle &= \begin{pmatrix}\cos\frac{\theta}{2}e^{-\mathrm{i}\phi} & \sin\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix}\begin{pmatrix}\sin\frac{\theta}{2}e^{-\mathrm{i}\phi}\\ -\cos\frac{\theta}{2}\end{pmatrix} \\
&= \mathrm{i}(\cos^2\frac{\theta}{2}e^{\mathrm{i}\phi} + \sin^2\frac{\theta}{2}e^{-\mathrm{i}\phi}) \\
&= \mathrm{i}\cos\phi - \sin\phi\cos\theta \\
\langle +|\sigma_z|-\rangle &= \begin{pmatrix}\cos\frac{\theta}{2}e^{-\mathrm{i}\phi} & \sin\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\sin\frac{\theta}{2}e^{-\mathrm{i}\phi}\\ -\cos\frac{\theta}{2}\end{pmatrix} \\
&= 0
\end{aligned}
$$

then

$$
\begin{aligned}
\langle +|\partial\mathcal{H}/\partial t|-\rangle &= -2\delta\omega\cos(\omega t)\sin(qa/2)\langle +|\sigma_y|-\rangle - \Delta\omega\sin(\omega t)\langle +|\sigma_z|-\rangle \\
&= -2\delta\omega\cos(\omega t)\sin(qa/2)(\mathrm{i}\cos\phi - \sin\phi\cos\theta)
\end{aligned}
$$

Thus the adiabatic condition reads

$$
\frac{2\delta\omega\cos(\omega t)\sin(qa/2)(\mathrm{i}\cos\phi - \sin\phi\cos\theta)}{2|\mathcal{E}(q,t)|} \ll \frac{|\mathcal{E}(q,t)|}{\hbar}
$$

approximately, this means that $\hbar\omega\cdot\delta \ll |\mathcal{E}(q,t)|^2$.

III. CONCLUTION

I think $\hbar\omega \ll$ the minimal energy scale (minimum of J,δ,Δ) is a good limit for adiabatic approximation.

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[1] Di Xiao, Ming-Che Chang, and Qian Niu, *Berry phase effects on electronic properties*, Rev. Mod. Phys. **82**, 1959 (2010).

[2] J. J. Sakurai, *Modern Quantum Mechanics, 2nd ed.*, Chap. 5, Sec.6 .