Topics

- Inclusion of initial correlations to linear response
  - Stationary susceptibility

    C.U.,Masaki Aihara, Mizuhiko Saeki, Seiji Miyashita, Phys. Rev. E80, 021128 (2009)

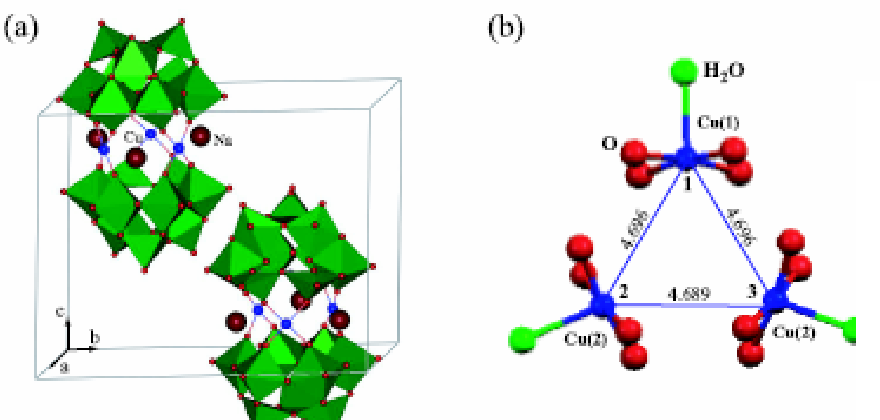
  - Transient linear response

    C.U.,Masaki Aihara, quant-ph/1008.2423, to be appeared in PRA

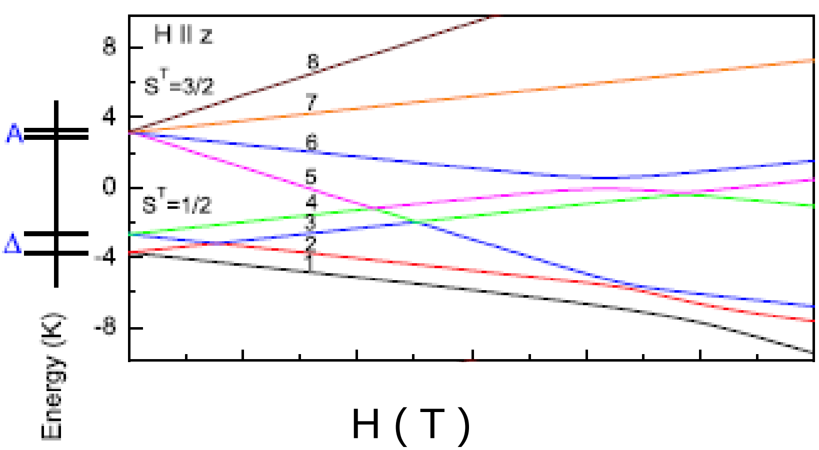
1.Backgrounds -1

Nanomagnet (nanoscale storing device)

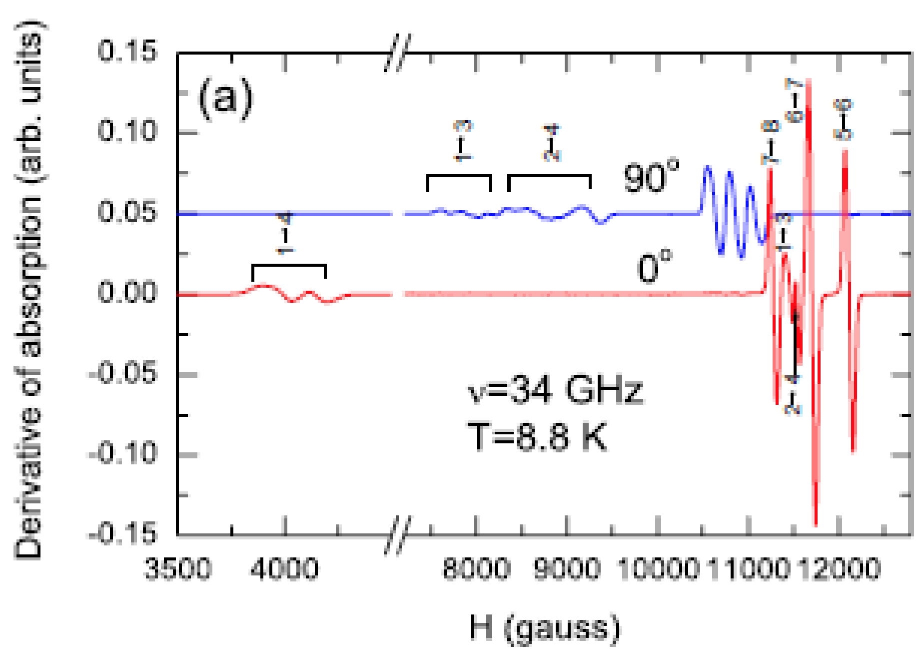
$\{Cu_3\}$ – type triangular spin ring



$Na_9[Cu_3Na_3(H_2O)_9(\alpha\text{-}AsW_9O_{33})_2]\cdot 26\ H_2O$



ESR experiment



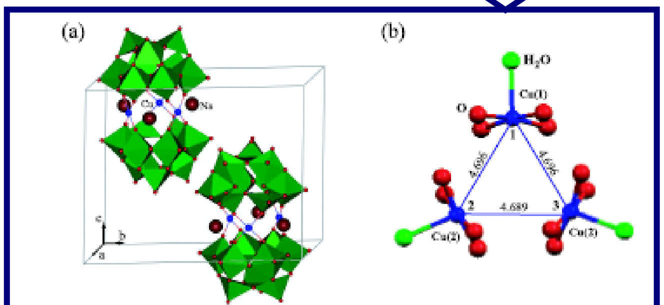
K-Y. Choi, et.al. PRL96(2006)107202

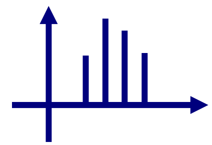
1.Backgrounds -2

Possible methods to obtain line shape

- Ensemble of eigenstates of total system

Dipolar broadening **Van Vleck(1948)**

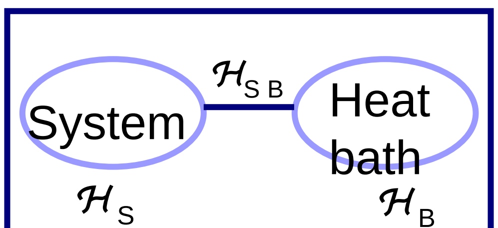




S. Miyashita, T. Yoshino and A. Ogasahara(1999)

We need
continuous line shape for
multiple spin systems!

- Projected state of relevant system coupled with bath



Bloembergen-Purcell-Pound(1947)
Bloch(1946,1953,1957)
Kubo-Tomita(1954), Kubo(1957)
Caldeira-Leggett(1987)

1.Backgrounds-3

Linear Response Theory

R.Kubo;JPSJ12(1957)570

Complex susceptibility

$$\chi_{\mu\nu}(\omega) = \lim_{\varepsilon\to 0}\int_0^\infty dt\ \ \Phi_{\mu\nu}(t)\, e^{-i\omega t-\varepsilon t}$$

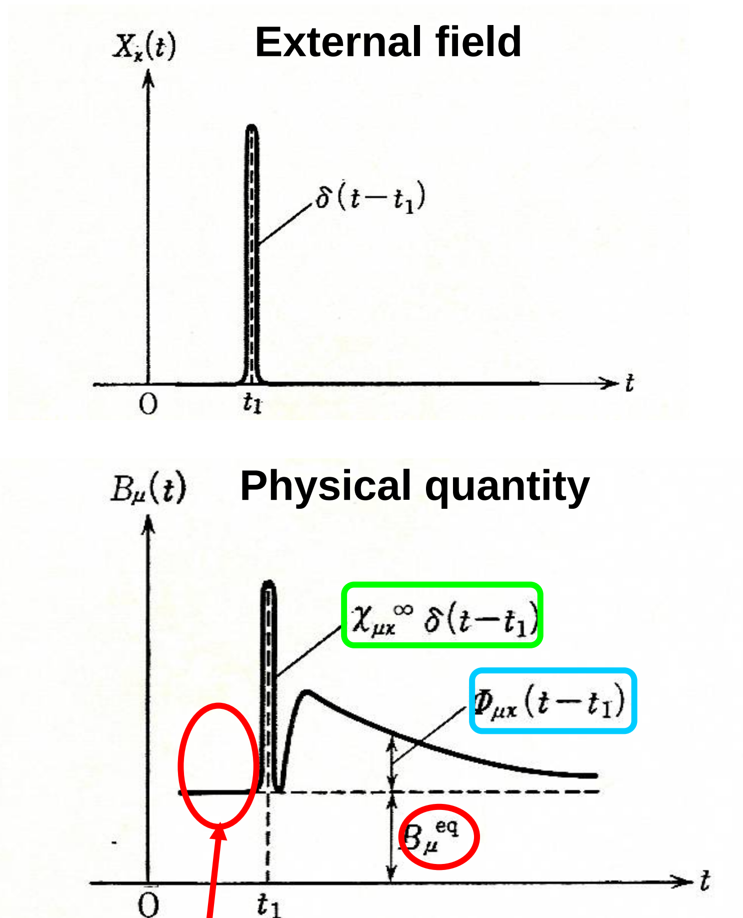
Response function

$$\Phi_{\mu\nu}(t) = \left\langle \frac{1}{i\hbar}\left[A_\nu, B_\mu(t)\right]\right\rangle$$

Response of an operator B_μ

to an external field $H(t) = -\sum_\nu X_\nu(t) A_\nu$

Definition of response function



frequently used assumption

relevant system stays in an equilibrium state

1.Backgrounds -4

Conventional treatments

Regression Theorem
L. Onsager, PR38(1931) 2265

$$\langle B_\mu(t) A_\nu \rangle \Leftarrow \langle B_\mu(t) \rangle$$

Guaranteed in Markovian approximation

M.Lax,PR172(1968)350;
F. Haake,PRA(1971)1723

This study

$$\Phi_{\mu\nu}(t) = \frac{i}{\hbar} \mathrm{Tr}_{S+B}\left[W^{eq} \left[B_\mu(t), A_\nu \right] \right]$$

Total system
(System + Bath)

In order to include initial correlation, non-Markovian approach is necessary

2.Objective of this study

- Quantum treatment of total system for an equilibrium state just before application of an external field

$$\Phi_{\mu\nu}(t) = \frac{i}{\hbar} Tr_s \left[\rho^{eq} \left[B_\mu(t), A_\nu \right] \right]$$

Only relevant system

$$\Phi_{\mu\nu}(t) = \frac{i}{\hbar} Tr_{S+B} \left[W^{eq} \left[B_\mu(t), A_\nu \right] \right]$$

Total system

- initial correlation
- temperature dependence
- extension to multiple spin system
- Non-Markovian effect

an analytic tool to characterize an environment surrounding spin microscopically

3.Formulation

Complex susceptibility

$$\chi_{\mu\nu}(\omega) = \frac{i}{\hbar}\int_0^\infty dt\, e^{-i\omega t}\, Tr_{S+R}\left[W^{eq}\left[B_\mu(t), A_\nu\right]\right] = \frac{i}{\hbar}\int_0^\infty dt\, e^{-i\omega t}\, Tr_S\left(B_\mu\, \rho_{A_\nu}(t)\right)$$

Time evolution of response function

$$\rho_{A_\nu}(t) = Tr_R\left\{e^{-i\mathcal{L}t}\left[A_\nu, W^{eq}\right]\right\}$$

Master eq. of $\rho_{A_\nu}(t)$

Damping theory

Memory term　　Inhomogeneous term

$$i\hbar\frac{d}{dt}\rho_{A_\nu}(t) = \mathcal{P}(-i\mathcal{L}_0)\rho_{A_\nu}(t) + \int_0^t d\tau\, \xi(t-\tau)\rho_{A_\nu}(\tau) + \mathcal{I}(t)[A_\nu, w^{eq}]$$

Uchiyama-Shibata PRE60(1999)2636

Fourier-LaplaceTransformation

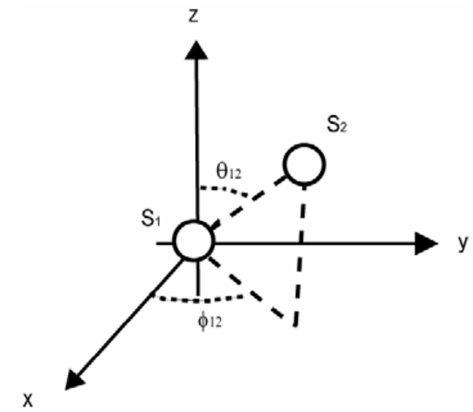
$$\chi_{\mu\nu}(\omega) = \frac{i}{\hbar}\mathrm{Tr}_S\left(B_\mu \frac{1}{-i\omega + i\mathcal{L}_S - \Xi[\omega]}\left(\rho_{A_\nu}(0) + \mathcal{I}_{A_\nu}[\omega]\right)\right)$$

Transformation to matrix

$$\chi_{\mu\nu}(\omega) = \frac{i}{\hbar}\left(\vec{B}_\mu, \frac{1}{-i\omega + i\mathcal{M}_S - \mathcal{M}_{\Xi_2}[\omega]}\left(\vec{\rho}_{A_\nu}(0) + \vec{\mathcal{I}}_{A_\nu}[\omega]\right)\right)$$

2^{nd} order of system-bath Interaction

4. Application to 2-spin system -1

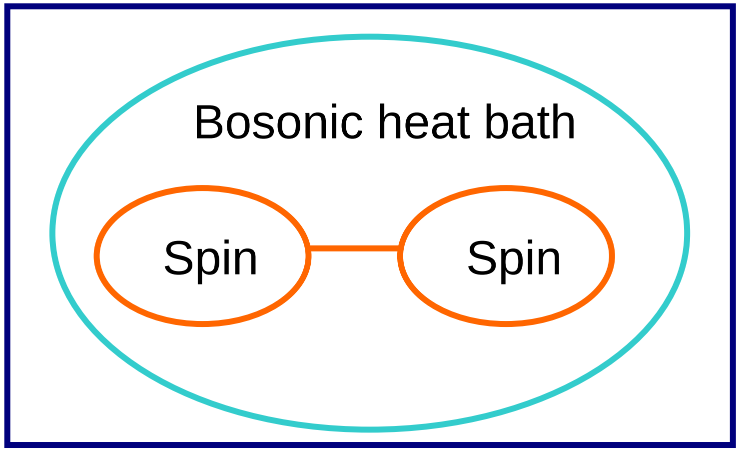


Relevant system

$$\mathcal{H}_S = \hbar\omega_0 \sum_{i=1}^{N} S_{i,z} + \mathcal{H}_{ex} + \mathcal{H}_D$$

$$\mathcal{H}_{ex} = -2J \sum_{i,j=1}^{N} (S_{i,+}S_{j,-} + S_{i,-}S_{j,+} + AS_{i,z}S_{j,z})$$

$$\mathcal{H}_D = D \sum_{i,j=1}^{N} \frac{1}{r_{ij}^3} \left\{ \mathbf{S}_i \bullet \mathbf{S}_j - \frac{3}{r_{ij}^2} (\mathbf{S}_i \bullet \mathbf{r}_{ij})(\mathbf{S}_j \bullet \mathbf{r}_{ij}) \right\}$$

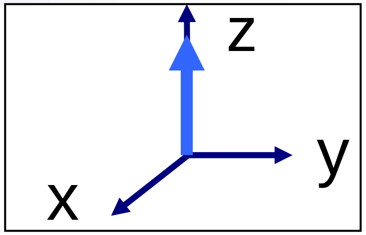


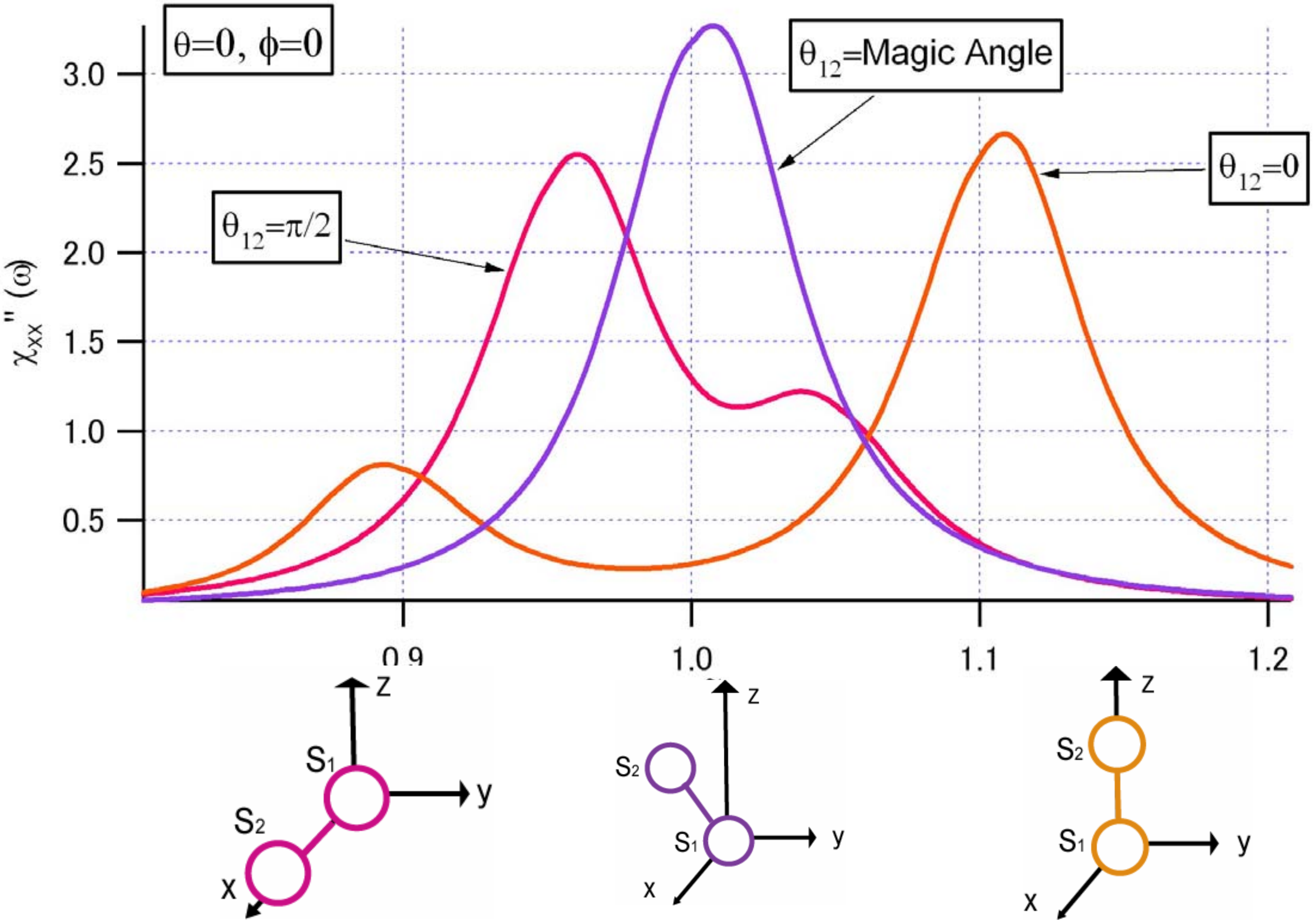
Sytem-bath interaction

$$\mathcal{H}_{SR} = \hbar \sum_n (aS_{n,-} + a^* S_{n,-} + cS_{n,z}) \sum_\alpha g_\alpha (b_\alpha^\dagger + b_\alpha)$$

$$I(\omega) = s\,\omega\, e^{-\omega/\omega_c}$$; ohmic spectral function, $n(\omega) = 1/(e^{\beta\hbar\omega} - 1)$

Pure dephasing $(a = 0,\ c = 1)$





$$k_B T = \hbar\omega_0$$

$$\tilde{\omega}_c = \frac{\omega_c}{\omega_0} = 0.5\ ,$$

$$s = \frac{1}{100}\ ,$$

$$\tilde{D}_0 = \frac{D_0}{\omega_0} = 0.1\ ,$$

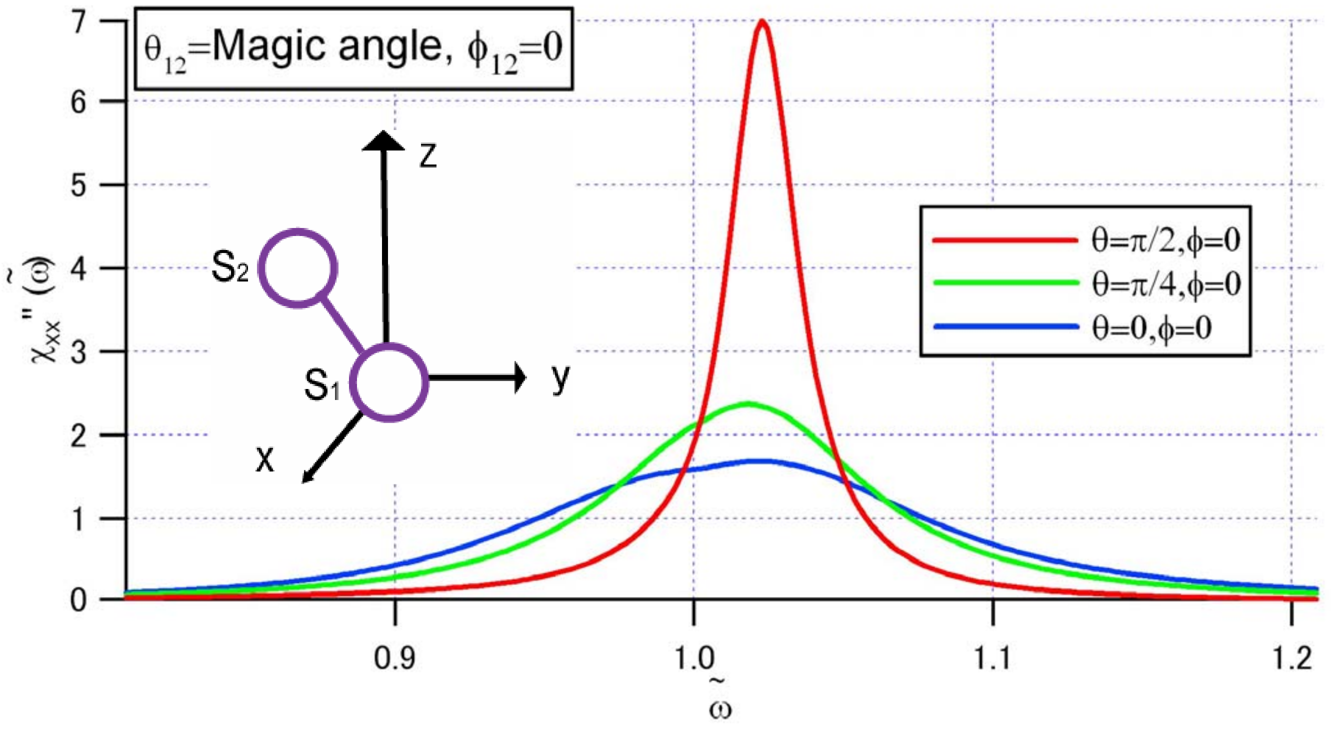
$$\tilde{J} = \frac{J}{\omega_0} = -1$$

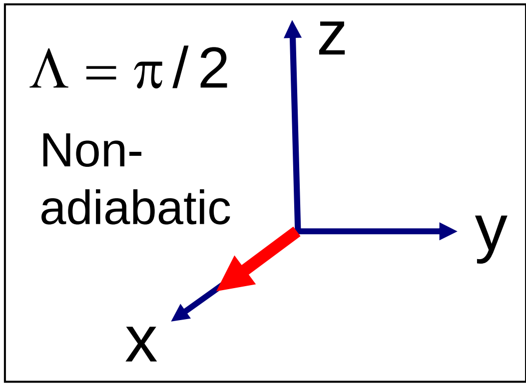
Demonstration of Nagata-Tazuke effect
(dependence of line shape on geometrical structure)

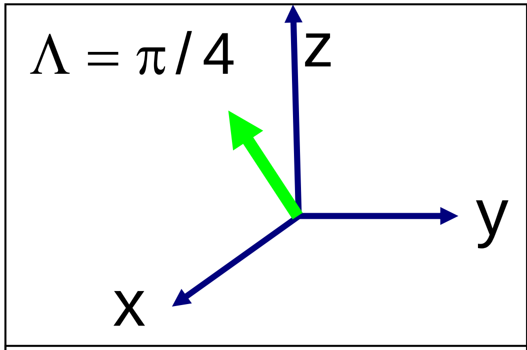
Effect of heat bath for magic angle case

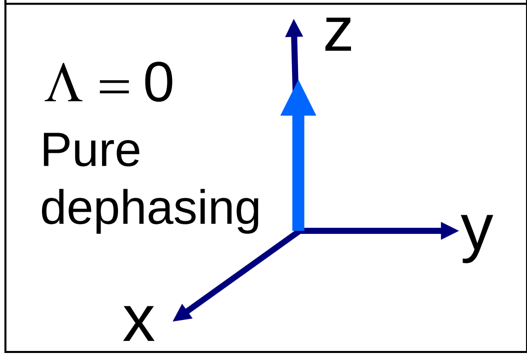
$$\mathcal{H}_{SB} = \hbar \ (aS_x + cS_z) \ \sum_{\alpha} g_\alpha (b_\alpha^\dagger + b_\alpha)$$

$$a = \sin\Lambda \ , \ c = \cos\Lambda$$

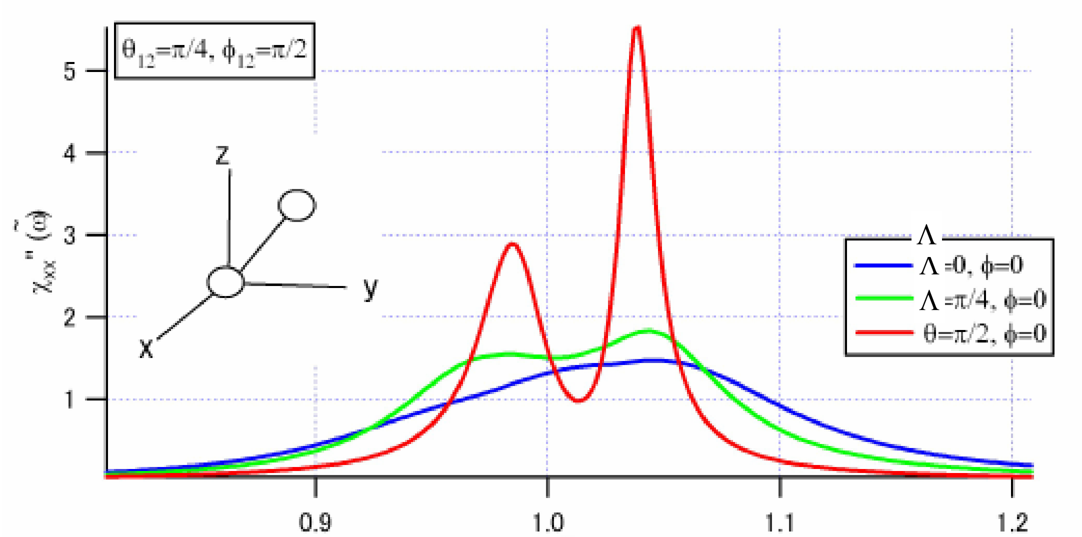


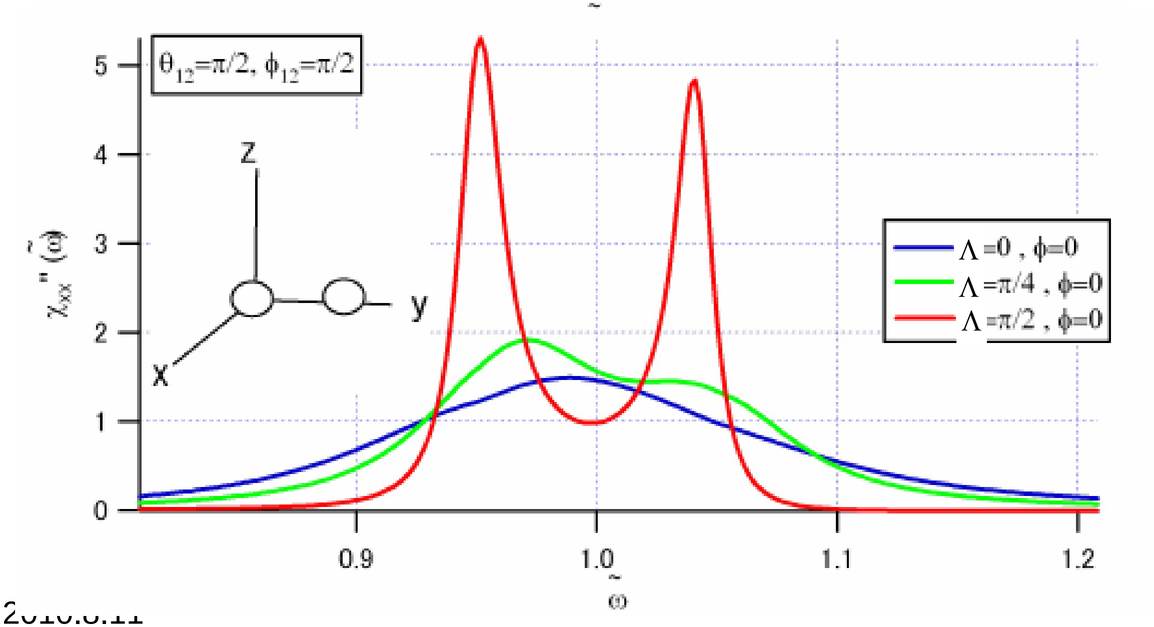


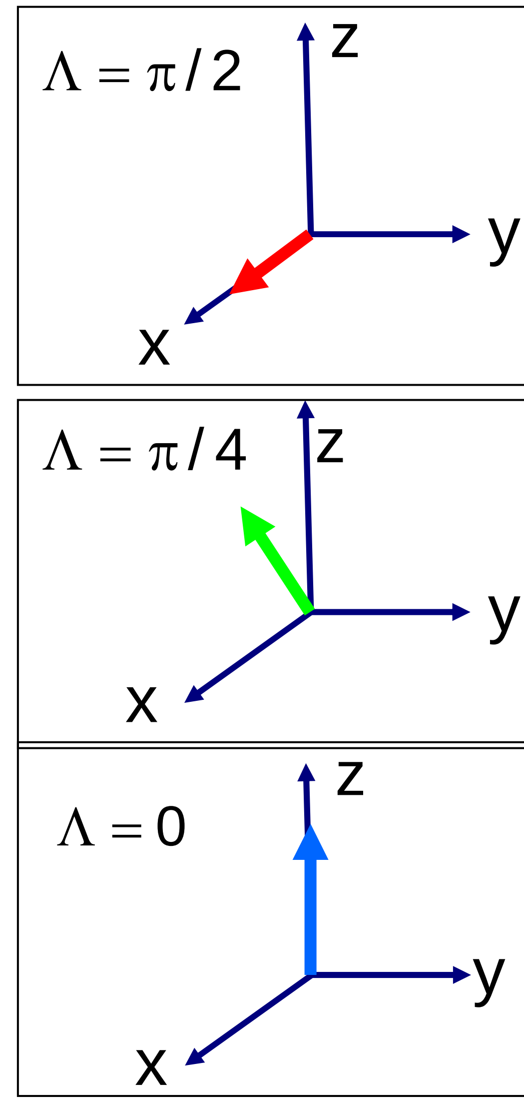




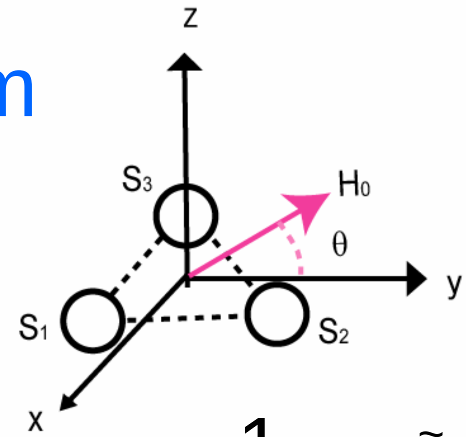
Effect of heat bath other than magic angle case

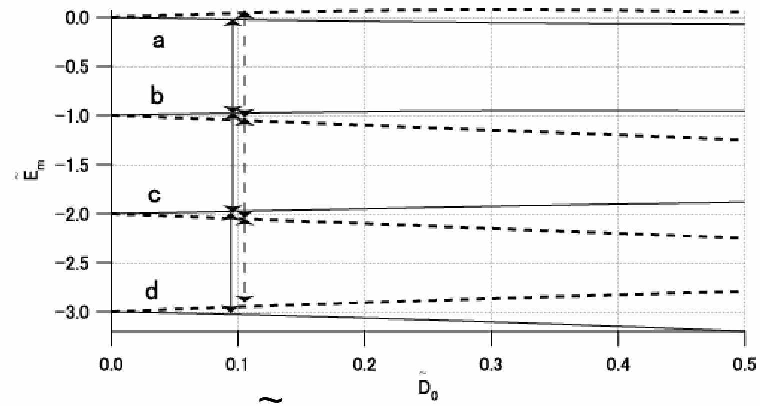




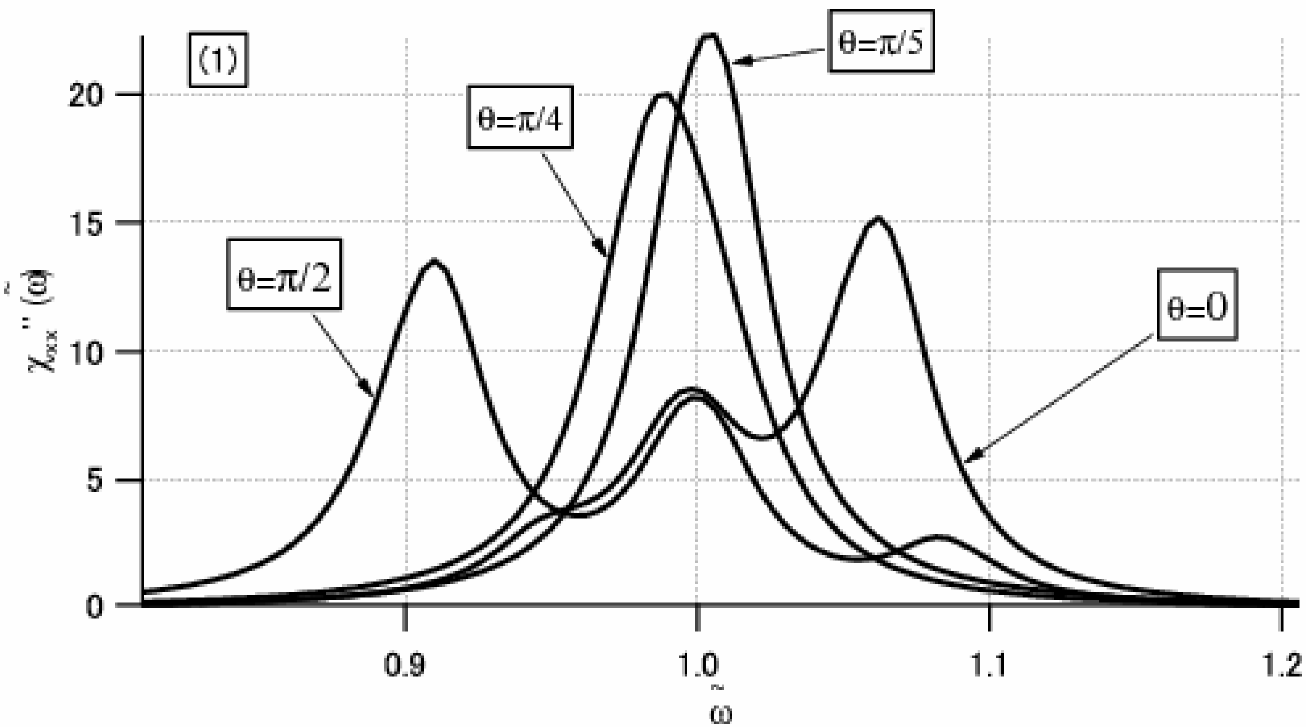


5. 3-spin system





$$\tilde{\omega}_c = \frac{\omega_c}{\omega_0} = 0.5\,,\quad s = \frac{1}{150}\,,\quad \tilde{D}_0 = 0.1\,, \tilde{J} = 1\,, k_B T = \hbar\omega_0$$



6. Conclusion

- Line shape theory for multiple spin system with including
  - System-environment interaction
    - initial correlation, frequency shift, non-Markovian effect
  - Interaction between spins among the relevant system
- Applicable to
  - arbitrary type of system-environment interaction
  - arbitrary number of spins
  - arbitrary geometrical structure of spins

Phys. Rev. E80, 021128 (2009)

Role of initial quantum correlation in transient linear response

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With Masaki Aihara, NAIST

quant-ph/1008.2423, to be appeared in PRA

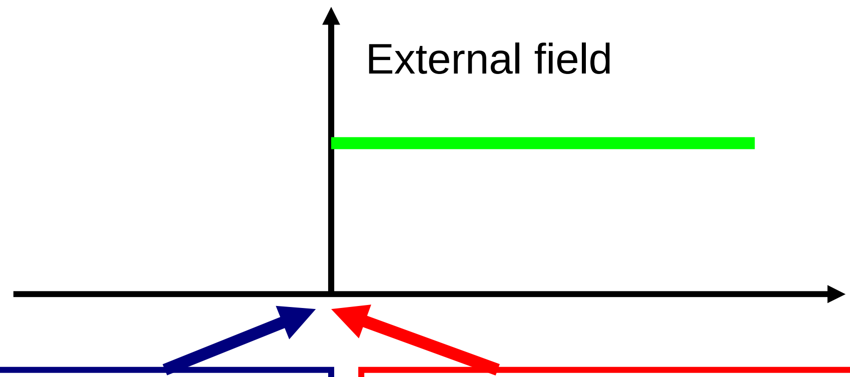
1.Motivation

- Effects of initial correlations
  - Quantum dynamics
    - under bosonic bath
    - under stochastic environment
  - Complete positivity of dynamical maps
  - Non-linear optical response

Do initial correlations affect on transient linear response?

2.Model -1

Transient linear response of an induced dipole moment



- Correlated initial condition

$$\rho(0) = \frac{1}{Z}\exp[-\beta\mathcal{H}]$$

equilibrium state of total system

- Factorized initial condition

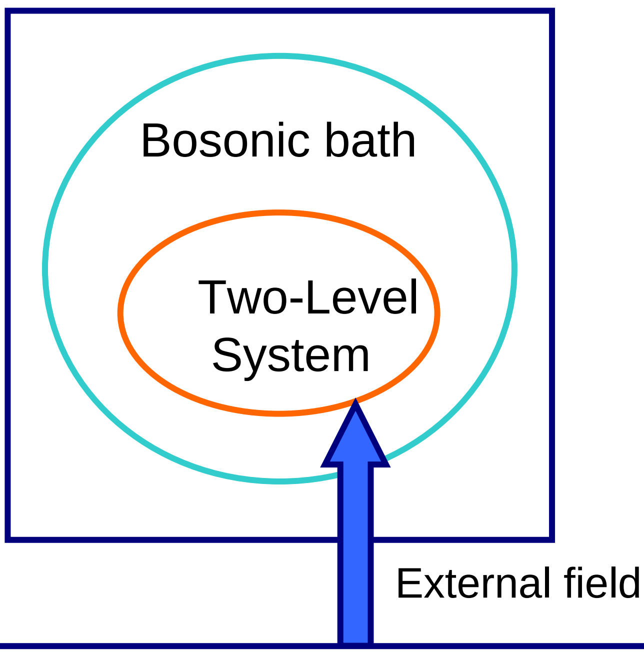
$$\rho(0) = \rho_s \otimes \rho_R$$

Separate equilibrium state

Can we find a difference between these cases?

2.Model-2

- Two-level system linearly and adiabatically coupled with a bosonic bath



$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_R + \mathcal{H}_{SR}$$

$$\mathcal{H}_S = E_1 |1\rangle\langle 1| + E_0 |0\rangle\langle 0|$$

$$\mathcal{H}_R = \sum_k \hbar\omega_k b_k{}^{\dagger} b_k$$

$$\mathcal{H}_{SR} = \sum_k \hbar g_k (b_k{}^{\dagger} + b_k) |1\rangle\langle 1|$$

$$\mathcal{H}_P(t) = -\frac{1}{2}\vec{\mu} \bullet \vec{E}\,\theta(t) |1\rangle\langle 0| e^{-i\omega_p t} + h.c.$$

3. Formulation-1

Case(1)
Correlated initial condition

$$\rho(0) = \frac{1}{Z}\exp[-\beta \mathcal{H}]$$

Case (2)
Factorized initial condition

$$\rho(0) = \rho_s \otimes \rho_R$$

$$canonical\ \ transformation: \ S = \exp[B|1\rangle\langle 1|], \quad B = \sum_k \frac{g_k}{\omega_k}(b_k - b_k^\dagger)$$

$$\rho'(0) = S^\dagger \rho(0) S = \rho_1 |1\rangle\langle 1| + \rho_0 |0\rangle\langle 0|$$

Separate state (Case (1))

$$\rho_1 = \frac{e^{-\beta E_1'}\rho_R}{Z_S'}, \quad \rho_0 = \frac{e^{-\beta E_0}\rho_R}{Z_S'}$$

$$E_1' = E_1 - \hbar \sum_k \frac{g_k^2}{\omega_k}$$

Shift

Correlated state (Case (2))

$$\rho_1 = \frac{e^{-\beta E_1}\rho_R'}{Z_S}, \quad \rho_0 = \frac{e^{-\beta E_0}\rho_R}{Z_S}$$

ρ_R' is a Gibbs state defined by

displacement

$$\mathcal{H}_R' = \sum_k \hbar\omega_k (b_k^\dagger - \frac{g_k}{\omega_k})(b_k - \frac{g_k}{\omega_k})$$

3. Formulation -2

- Induced dipole moment

$$\mu_{(m)}(t) = \left|A_{(m)}(t)\right| \cos(\omega_p t + \phi_{(m)}(t)), \qquad (m = 1, 2)$$

Correlated i.c.

$$A_{(1)}(t) = \frac{1}{Z_S'} \int_0^t dt' e^{i\Delta\omega(t-t')} \left\{ e^{-\beta E_1'} \Psi_1(t-t') - e^{-\beta E_0} \Psi^*{}_1(t-t') \right\}$$

Factorized i.c.

$$A_{(2)}(t) = \frac{1}{Z_S} \int_0^t dt' e^{i\Delta\omega(t-t')} \left\{ e^{-\beta E_1} \Psi_2(t,t') - e^{-\beta E_0} \Psi^*{}_1(t-t') \right\}$$

$$\Delta\omega = \omega_p - (E_1' - E_0)/\hbar$$

for Ohmic spectral function

$$\Psi_1(t) = \exp[-\xi(t) - i\, s \arctan(\omega_c t)] \;, \xi(t) = \int_0^\infty \frac{h(\omega)}{\omega^2}(1 + 2n(\omega))(1 - \cos(\omega t))$$

$$\Psi_2(t,t') = \Psi_1(t - t') \exp[-2i\, s (\arctan(\omega_c t') - \arctan(\omega_c t))]$$

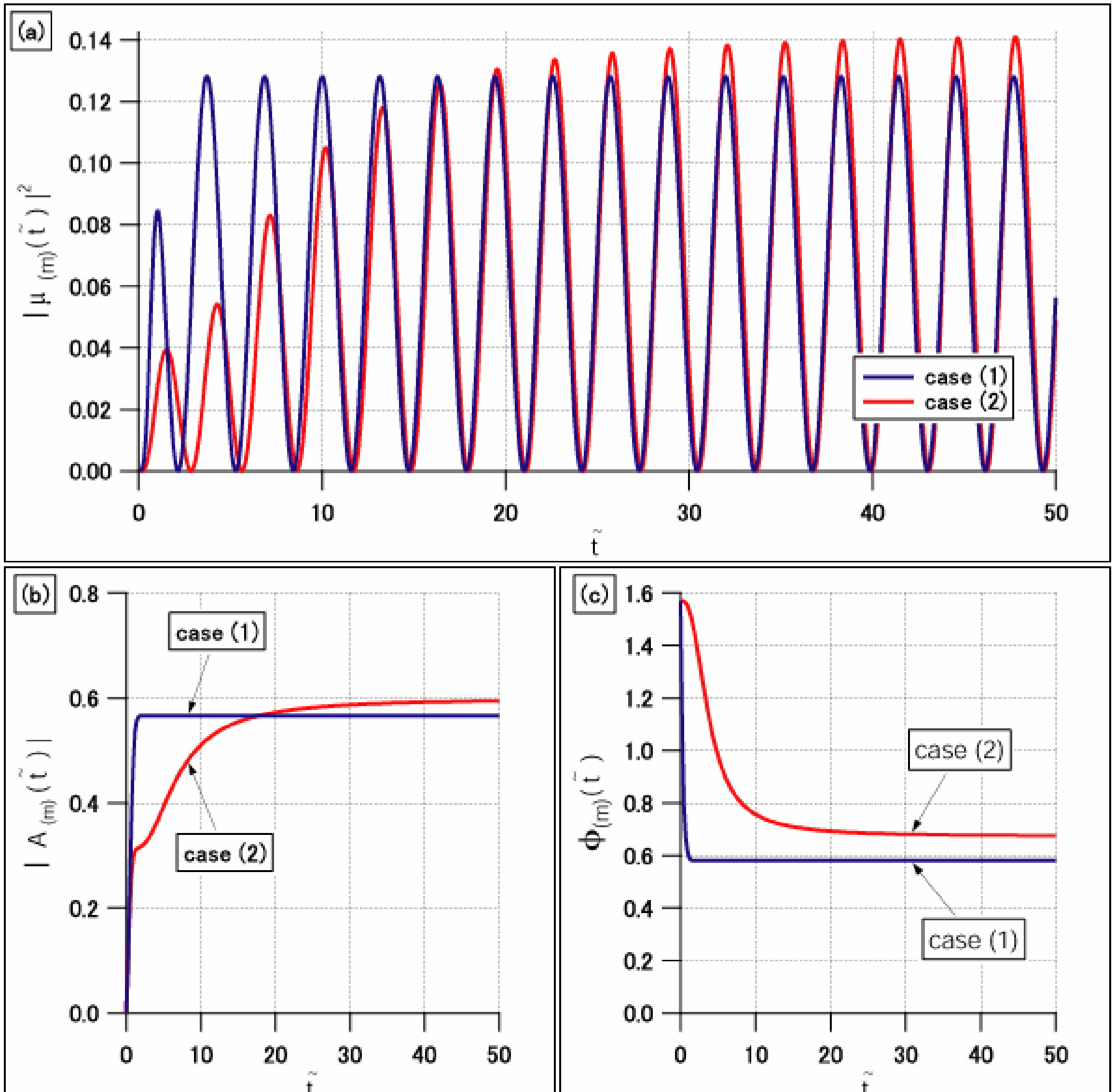
4. Numerical Evaluations

Ohmic spectral function

$$k_B T = 10\hbar\omega_0$$

$$s = 1$$

$$\omega_c = \omega_0 / 5$$

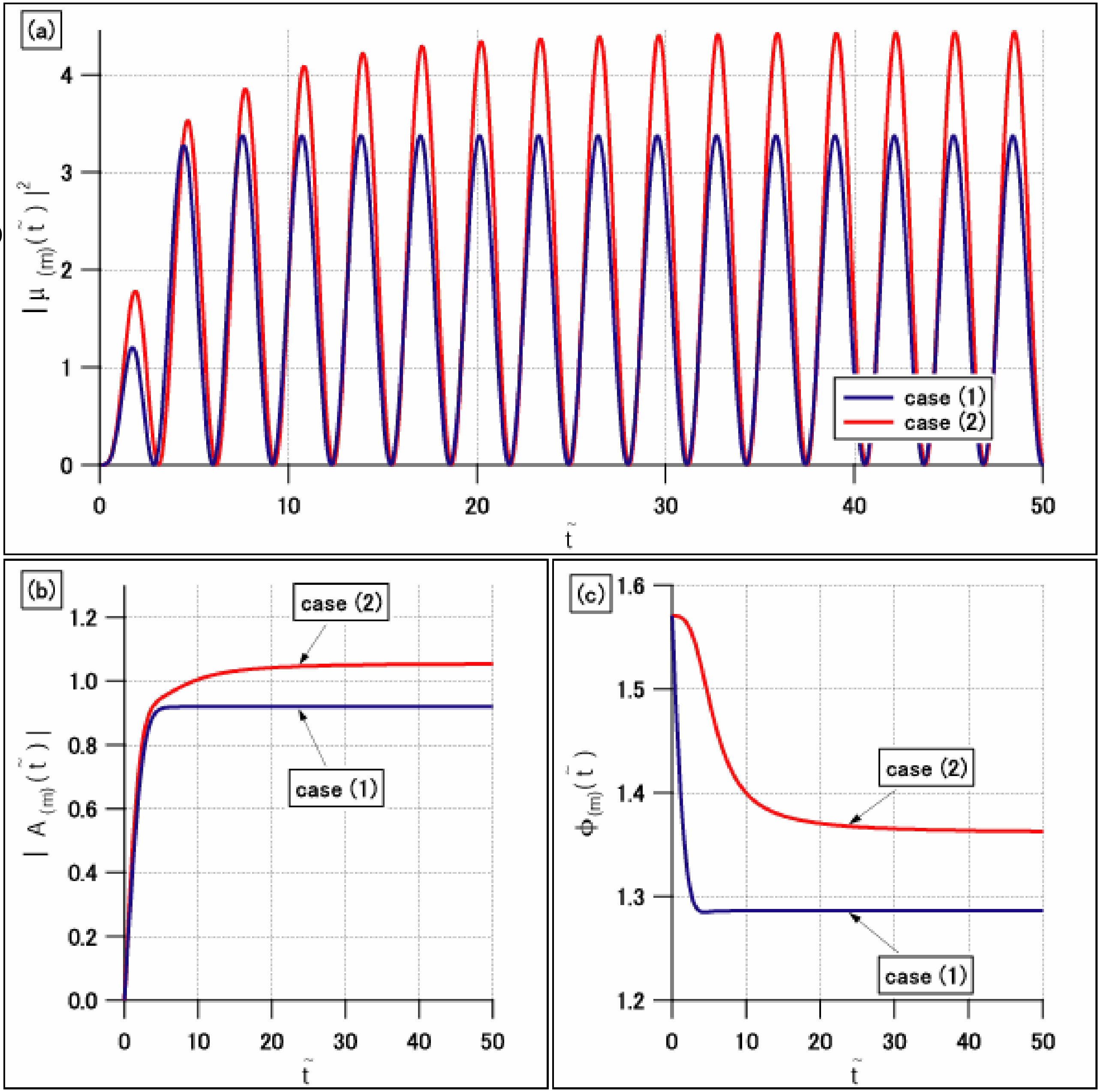


Case (1)
Correlated i.c.
Case(2)
Factorized i.c.

$$k_B T = \hbar\omega_0$$

$$s = 1$$

$$\omega_c = \omega_0 / 5$$

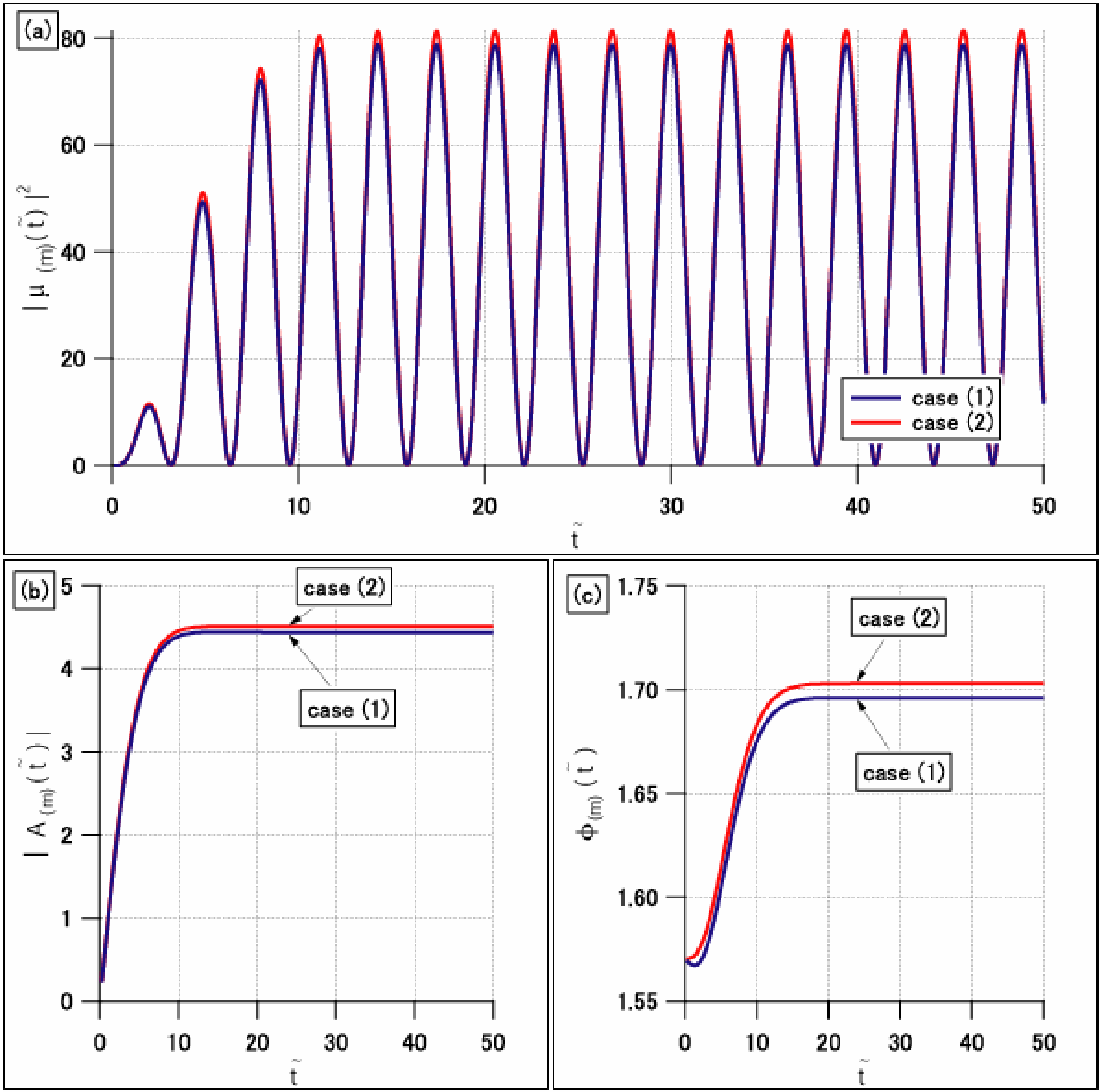


Case (1)
Correlated i.c.
Case(2)
Factorized i.c.

$$k_B T = \hbar\omega_0 / 5$$

$$s = 1$$

$$\omega_c = \omega_0 / 5$$



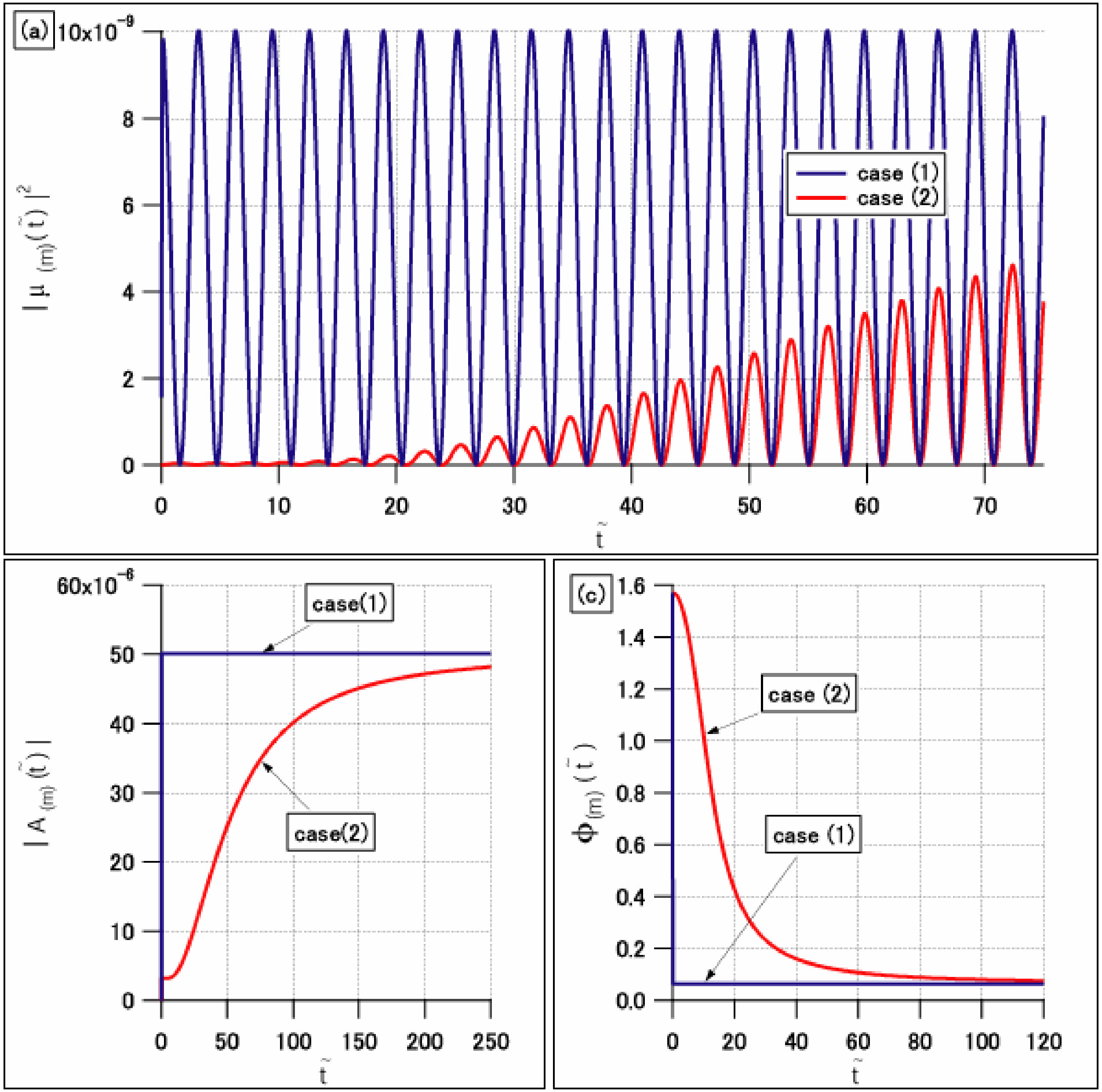
Case (1)
Correlated i.c.
Case(2)
Factorized i.c.

High-temperature case

$k_B T = 10^4\,\hbar\omega_0$

$s = 1$

$\omega_c = \omega_0 / 50$



Case (1)
Correlated i.c.
Case(2)
Factorized i.c.

5. Conclusion

- Factorized initial condition (separate equilibrium state) can make an artifact in transient linear response.
  - Overestimation
  - Phase shift

  } **•Intermediate temperatures**
  •Strong system-environment coupling

- Future study
  - Non-linear response
  - Extension to multiple two-level systems

C.U.,Masaki Aihara, quant-ph/1008.2423, to be appeared in PRA