Tutorial on how to solve the Liouville equation for Many Body Systems:

Mori-Lee Theory/Projection Operator Technique

Surajit Sen

Physics Dept, SUNY-Buffalo

Outline

1. What is often needed …
2. Formal Solution to Liouville Eq. (LE)
3. Implicit Assumptions
4. Recurrence Relations
5. Continued Fractions

1. **What is often needed** for many body systems that can be experimentally probed using scattering techniques?

Dynamical Response Functions (DRF) – Linear response to “weak” perturbation

e.g., $\chi(\mathbf{k}, \omega, T)$ – Dynamic Susceptibility

$S(\mathbf{k}, \omega, T)$ – Dynamic Structure Factor

k = momentum, ω = frequency, T = temperature

Typically, total no. of particles N is large enough such that thermodynamic limit can be assumed

Theoretical starting point –

Define Hamiltonian $H(=H^{+})$ and some $A(t)$, solve LE

$dA(t)/dt = iLA(t)$, $L = (1/\hbar)[H, \,]$ (Quantum Systems), $L = \{,H\}$ (Classical Systems)

LE leads to $A(t)$

Typically, $_0\int^{\infty} dt \exp(i\omega t)(A(t),A(0))/(A,A) \rightarrow$ DRF,

T enters via Kubo’s “Fluctuation-Dissipation Theorem” (1957/1966)

(X,Y) is some “scalar product” like the fluctuation formula, susceptibility formula, etc

$(X,Y)=\langle XY\rangle-\langle X\rangle\langle Y\rangle$, or $(X,Y) = (1/\beta)_0\int^{\beta} d\lambda \langle \exp(\lambda H)X\exp(-\lambda H)Y^{+}\rangle-\langle X\rangle\langle Y^{+}\rangle$

2. Formal solution to LE

$A(t) = \exp(iHt)A(t=0)\exp(-iHt)$ (commutation must be done to evaluate this ..)

- now do a short time (or equivalently, high frequency) expansion

- but expansion does not solve for A(t) for ALL times – so low frequency information remains hard to get

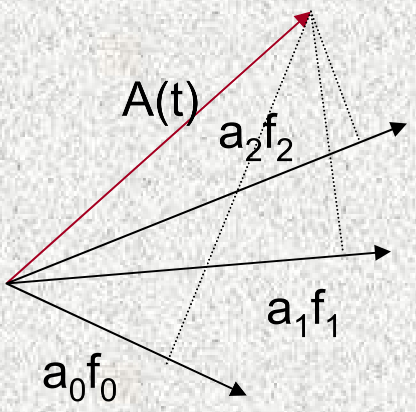
Mori-Lee/Projection operator approach to solving LE (whole point is to get long time/low frequency dynamics)

$A(t) = \sum_{\nu=0}^{d-1} a_\nu(t,\beta)\, f_\nu(\beta)$

Now find $\{f_\nu(\beta)\}$ and $\{a_\nu(t,\beta)\}$

Orthogonal Operators (sort of like normal modes)

Time-dependent correlations



How to make f_ν orthogonal? Must define a scalar product for the vector space in which f_ν lives … Kubo scalar product

$$(X,Y) = (1/\beta)\int_0^\beta d\lambda \langle \exp(\lambda H)X\exp(-\lambda H)Y^+\rangle - \langle X\rangle\langle Y^+\rangle$$

3. Implicit Assumptions (remember, Mori-Lee is an exact approach, but there are conditions to be kept in mind)

1. System under study (characterized by $H=H^+$) lives in a heat bath described via the canonical ensemble [Can this be relaxed? Open question]
2. Ergodicity is somehow implicit – A(t) can be oscillatory ⇒ system returns to some “original” perturbed state ⇒ perfect ability to remember/perfect memory ⇒ perturbation energy remains trapped ⇒ non-ergodic system.
3. But non-ergodic system still remains in contact with a (canonical ensemble) heat bath and this is not a realistic assumption
4. Assumption is that system must eventually return to a unique equilibrium state. Techniques have not been developed yet to handle metastable or arrested states. This is an open area.
5. H must be time independent – so driven systems can’t be treated

To deal with driven systems/get away from canonical ensemble assumptions, etc. the current state of the art (other than simulations) is mean-field theory type approaches with harmonic approximations or purely *ad-hoc* approaches!

4. Recurrence Relations (Heart of Mori-Lee/Projection Operator Theory)

1. Set A(t=0) = A
2. Now define a suitable scalar product (Kubo scalar product may be unnecessarily complicated, … keep this simple)
3. Now construct $\{f_\nu(\beta)\}$
4. Plug $\{f_\nu(\beta)\}$ into $A(t) = \sum_{\nu=0}^{d-1} a_\nu(t,\beta)\, f_\nu(\beta)$
5. Plug A(t) into LE,
6. Construct $\{a_\nu(t,\beta)\}$

Construction of $\{f_\nu(\beta)\}$ – Recurrence Relation I

$f_{\nu+1}(\beta) = iLf_\nu(\beta) + \Delta_\nu f_{\nu-1}, \ \nu\geq 1$

$f_1 = iLf_0$

Where $\Delta_\nu = (f_\nu, f_\nu)/(f_{\nu-1}, f_{\nu-1})$

Now use $\{f\nu(\beta)\}$ – Recurrence Relation I to get $\{a_\nu(t,\beta)\}$

One gets $\Delta_{\nu+1}\, a_{\nu+1}(t) = -da_\nu(t)/dt + a_{\nu-1}(t)$

$a_{-1} = 0$

Recurrence Relation II

Bad equation to solve because one must know $a_1(t)$ to find $a_0(t)$, etc. So, one must solve for all a_ν simultaneously!!

An important observation

Recall, $A(0) = f_0 \Rightarrow a_0 = 1,\ a_\nu = 0,\ \nu > 0$

$\Delta_1\, a_1(0) = -da_0(0)/dt = 0$

So, $da_0(0)/dt = 0 \Rightarrow$ Purely exponential functions can't be exact solutions to relaxation processes in Hermitian systems $\Rightarrow$ What looks like Lorentzian peaks of relaxation processes are not truly Lorentzian!

(Lee, PRL, 51, 1227 1983)

Reviews

A.S.T. Pires, Helv. Phys. Acta, 61, 988 (1988);

M.H. Lee, Comput. Physics Commun. 53, 147 (1989)

D. Vitali and P. Grigolini, Phys Rev A 39, 1486 (1989).

5. Continued Fractions – How to Solve Recurrence Relation II

Laplace Transform

$a_0(z) = {}_0\int^{\infty} dt \exp(-zt)a_0(t)$

Laplace Transform of both sides of RR II yields,

$a_0(z) = 1/(z + \Delta_1/(z + \Delta_2/(z + \Delta_3/(z + \Delta_4/(z + \dots$ (to (d-1) levels)))))

(continued fraction)

Now one can take an Inverse Laplace Transform of $a_0(z)$ to get

$a_0(t) = (1/2\pi i)\int_c dz \exp(zt)a_0(z)$

$$\downarrow$$

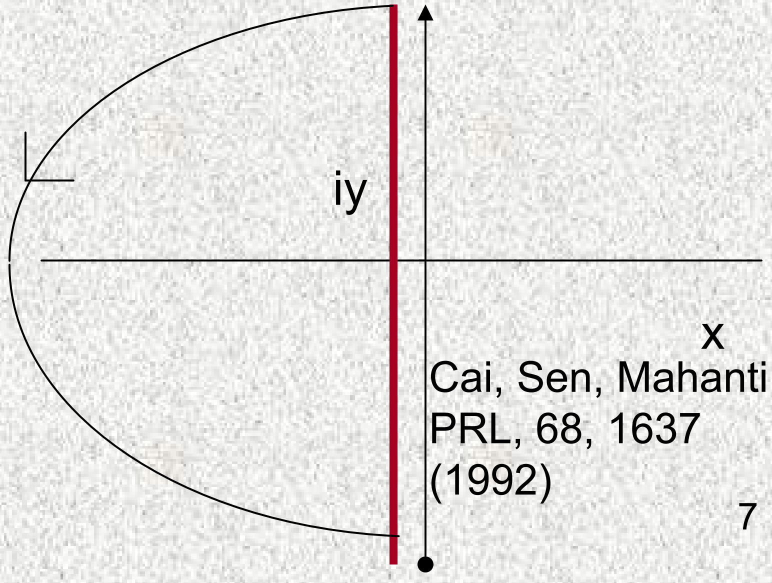
Usually tough to do

Cont fraction can be expanded in 1/z,

$a_0(z) = 1/z - \Delta_1/z^2 + (\Delta_1+\Delta_2)/z^3 - \dots$

$a_0(t) = 1 - \Delta_1 t^2 + (\Delta_1+\Delta_2)t^4 - \dots$

(even series in t)



Cai, Sen, Mahanti, PRL, 68, 1637 (1992)

If Δ_ν is a finite set, then the system is non-ergodic (in a canonical ensemble) – This is perhaps not that interesting within the context of Mori-Lee theory

[Sen, Proc. R Soc A 441, 169 (1993), Florencio et al, J. Phys A 22, L331 (1989)]

How do the Δ_ν grow with ν?

For most interacting many body systems one finds

$\Delta_\nu \sim \nu^\alpha$, where $0 \leq \alpha \leq 1$

Why so? Not known.

If $\alpha>2$, the continued fractions representations become “sensitive” in the sense that ALL poles must be accounted for to correctly obtain $a_0(t)$. This is the dynamical version of Yang-Lee theorem [Sen, Physica A 315, 150 (2002)]

Fast growth in Δ_ν - Case of the Quartic Oscillator in a Canonical Ensemble –

possible connection with critical dynamics in Ginzburg-Landau approach

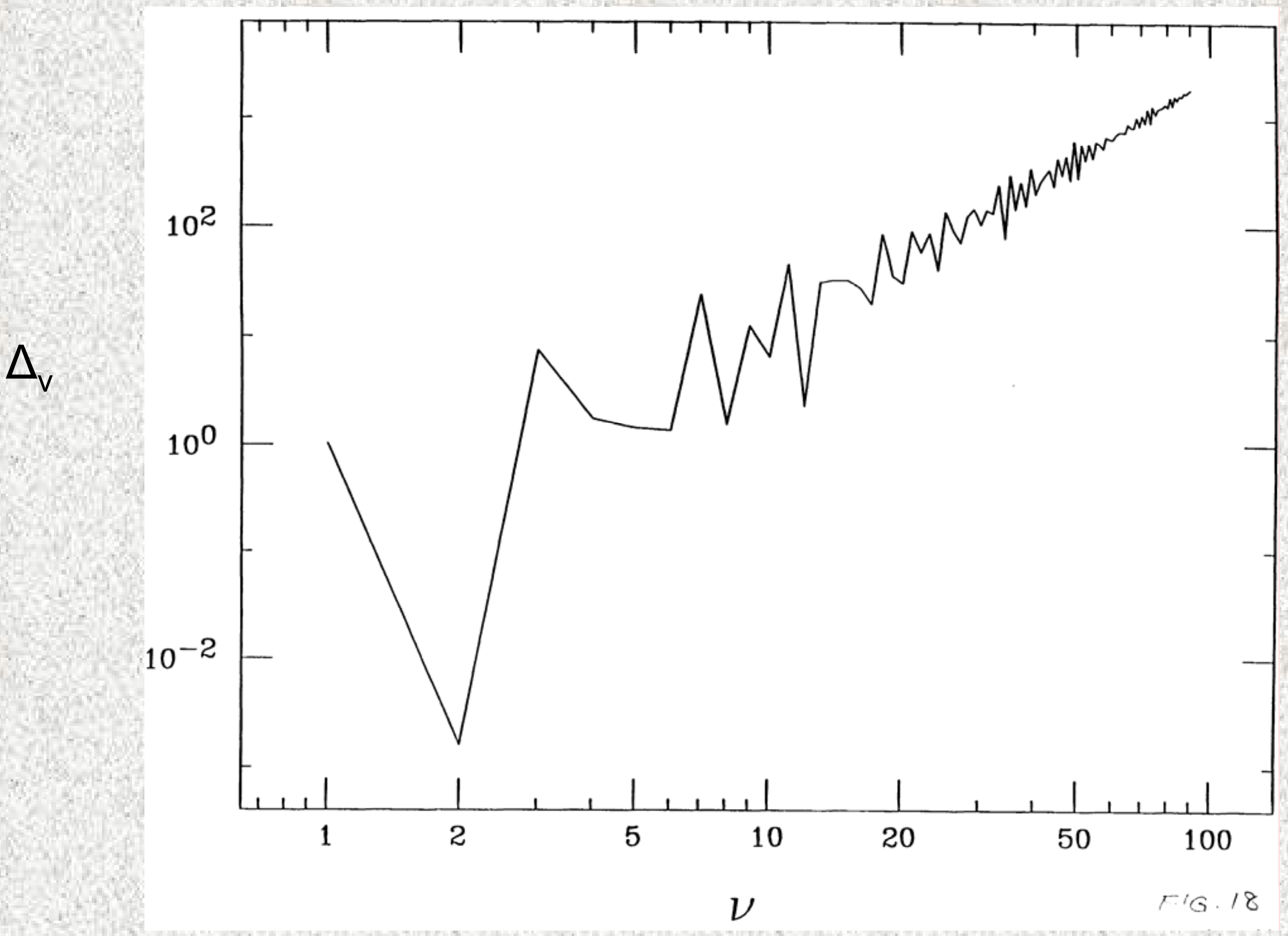


FIG. 18

Plot of Δ_v versus v for $\beta=100$ in a system with $V(x) = (x^2/2) + (x^4/4)$. In the case shown below $\Delta_\nu \sim \nu^{2.5}$.

Summary

- Mori-Lee/Projection Operator Theory

- started by Zwanzig (1959), formalized by Mori (1965), using Kubo's Fluctuation-Dissipation theorem (1957), Dupuis (1967), Lee (1982), Grigolini (1983)

- Present focus is on ergodic systems in canonical ensembles, find $\{\Delta_\nu\}$

- Calculate $a_0(z)$, Inverse Laplace Transform to $a_0(t)$, Fourier Transform to DRF

- Systems Solved:

Transverse Ising – 1D, 2D ($T=\infty$,0 in 1D, $T=\infty$ in 2D)

XY ($s=1/2$) – 1D ($T=0$, $T=\infty$)

Including Impurity Models

Heisenberg ($s=1/2$) – 1D ($T=\infty$ mostly)

Electron Gas (2D, 3D, Interacting cases at $T=0$)

Harmonic Oscillator Chains