Homework No.7, 550.695, Due April 30, 2009.

1. This problem discusses the dynamics for a 3-vector $(\widetilde{X}_1, \widetilde{X}_2, \widetilde{X}_3)$ defined by the Langevin equations

$$\dot{\widetilde{X}}_i = A_i \widetilde{X}_j \widetilde{X}_k - \nu_i \widetilde{X}_i + \widetilde{F}_i(t), \quad i = 1, 2, 3 \qquad (*)$$

driven by Gaussian white-noise forces $\widetilde{F}_i(t)$ with zero means and covariances

$$\langle \widetilde{F}_i(t) \widetilde{F}_j(t') \rangle = 2\kappa_i \delta_{ij} \delta(t - t').$$

Here (i, j, k) represents any cyclic permutation of $(1, 2, 3)$, $A_i,\ i = 1, 2, 3$ are real numbers satisfying

$$A_1 + A_2 + A_3 = 0,$$

and $\nu_i,\ \kappa_i,\ i = 1, 2, 3$ are positive real numbers. We shall employ the constants

$$A_1 = 2, A_2 = A_3 = -1,$$

$$\kappa_1 = 0.5, \kappa_2 = \kappa_3 = 0.1,$$

$$\nu_1 = 0.1, \nu_2 = \nu_3 = 0.5.$$

Mode 1 is a linearly unstable mode which is strongly forced and weakly damped, while modes 2 & 3 are linearly stable modes that are weakly forced and strongly damped. A nonlinear transfer of energy

$$E(t) = \frac{1}{2}[\widetilde{X}_1^2(t) + \widetilde{X}_2^2(t) + \widetilde{X}_3^2(t)]$$

develops, on average, from mode 1 into modes 2 & 3.

(a) Use a direct ensemble method to study the statistical dynamics of this system. Take $\widetilde{X}_1(0), \widetilde{X}_2(0), \widetilde{X}_3(0)$ to be independent normal random variables with zero means and variances

$$\langle \widetilde{X}_1^2(0) \rangle = 0.8, \langle \widetilde{X}_2^2(0) \rangle = \langle \widetilde{X}_3^2(0) \rangle = 0.6$$

and evolve an ensemble of $N = 10^4$ samples by the Euler-Maruyama scheme with $dt = 10^{-4}$ to calculate

$$M_i(t) = \langle \widetilde{X}_i^2(t) \rangle,\ i = 1, 2, 3, \qquad T(t) = \langle \widetilde{X}_1(t) \widetilde{X}_2(t) \widetilde{X}_3(t) \rangle,$$

for $0 < t < 1$. Record these results and the total CPU time.

(b) Show that the exact equations satisfied by the above moments are

$$\dot{M}_i = 2A_iT - 2\nu_iM_i + 2\kappa, \quad i = 1,2,3$$

$$\dot{T} = Q - (\nu_1 + \nu_2 + \nu_3)T$$

where Q is a 4th-order (quartic) moment defined by

$$Q = A_1\langle \widetilde{X}_2^2\widetilde{X}_3^2\rangle + A_2\langle \widetilde{X}_1^2\widetilde{X}_3^2\rangle + A_3\langle \widetilde{X}_1^2\widetilde{X}_2^2\rangle$$

Show that the solutions of the SDE (*) are invariant under pairwise reflections: $(\widetilde{X}_1, \widetilde{X}_2, \widetilde{X}_3) \longrightarrow (\widetilde{X}_1, -\widetilde{X}_2, -\widetilde{X}_3)$ and cyclic permutations. If the random initial conditions are statistically invariant under these same reflections, then this symmetry must therefore be preserved in time. Use this fact to argue that $\langle \widetilde{X}_i\widetilde{X}_j\rangle = 0$ for $i \neq j$, with the initial conditions considered in (a). Deduce from this that the *quasinormal closure (QN)* for the system corresponds to the exact equations for $M_i,\ i = 1,2,3$ and the following equation for T :

$$\dot{T} = A_1M_2M_3 + A_2M_1M_3 + A_3M_1M_2 - (\nu_1 + \nu_2 + \nu_3)T.$$

Solve the QN closure equation with initial conditions $M_1(0) = 0.8, M_2(0) = M_3(0) = 0.6, T(0) = 0$ using the Euler scheme with $\Delta t = 10^{-2}$ for $0 < t < 1$. Compare the closure results with the results of the direct ensemble method in terms of quantitative accuracy and computational efficiency.

(c) Let $N_i, N_i',\ i = 1,2,3$ be six i.i.d. $N(0,1)$ random variables. Define a set of "statistical surrogates"

$$\widetilde{Y}_i = \beta_i\widetilde{N}_i + \beta_4\widetilde{N}_j'\widetilde{N}_k'$$

for the variables $\widetilde{X}_i,\ i = 1,2,3$ with again (i,j,k) a cyclic permutation of $(1,2,3)$. Show that

$$M_i = \langle \widetilde{Y}_i^2\rangle = \beta_i^2 + \beta_4^2, \quad T = \langle \widetilde{Y}_1\widetilde{Y}_2\widetilde{Y}_3\rangle = \beta_4^3,$$

and for $i \neq j$

$$\langle \widetilde{Y}_i^2\widetilde{Y}_j^2\rangle = M_iM_j + 2\beta_4^4.$$

Use the above results to show that the QN closure for the 3-mode dynamical system (*) is realized by this statistical model, as long as $|T|^{2/3} < M_i$ for $i = 1,2,3$.

Exploit this statistical model to implement the QN closure in the 3-mode system by the *equation-free method.* Solve the closure equations as before using the Euler method with $\Delta t = 10^{-2}$ but evaluate the derivatives of the moment-variables using

$$\dot{\widetilde{\psi}}(t) \doteq \frac{\widetilde{\psi}(t+\delta t) - \widetilde{\psi}(t)}{\delta t},$$

with $\delta t = 10(dt) = 10^{-3}$ and then average over $N = 10^4$ samples to obtain the closure dynamics at each time-step. Compare with the previous two methods for accuracy and computational efficiency.

2. This problem involves the Rayleigh-Ritz/PDF-closure method of solving either the Schrödinger equation or the forward probability equation. Each of the following papers applies this method to a complex system with many degrees of freedom:

[1] R. P. Feynman and M. Cohen, "Energy spectrum of the excitations in liquid helium," Phys. Rev. **102** 1189–1204 (1956)

[2] J. Bardeen, L. N Cooper, and J. R. Schrieffer, "Theory of superconductivity," Phys. Rev. **108** 1175-1204 (1957)

[3] L. McMillan, "Ground state of liquid ^{4}He," Phys. Rev. A **138** 442–451 (1965)

[4] H. J. Kushner, "Approximations to optimal nonlinear filters," IEEE Trans. Automatic Control, **AC-12** 546–556 (1967)

[5] E. J. Heller, "Time-dependent approach to semiclassical dynamics," J.Chem. Phys. **62** 1544–1555 (1975)

[6] R. B. Laughlin, "Anomalous quantum Hall effect — An incompressible quantum fluid with fractionally charged excitations," Phys. Rev. Lett. **50** 1395–1398 (1983)

[7] R. H. Kraichnan, H. Chen, and S. Chen, "Probability distribution of a stochastically advected scalar field," Phys. Rev. Lett. **63** 2657–2657 (1989); Y. Kimura and R. H. Kraichnan, "Statistics of an advected passive scalar," Phys. Fluids A **5** 2264–2277 (1993)

[8] J. Ma, D. Hsu and J. E. Straub, "Approximate solution of the classical Liouville equation using Gaussian phase packet dynamics: Application to enhanced equilibrium averaging and global optimization," J. Chem. Phys. **99** 4024–4035 (1993)

[9] R. H. Kraichnan and T. Gotoh, "Statistics of decaying Burgers turbulence," Phys. Fluids A **5** 445–457 (1993)

[10] C. Yeung, Y. Oono, and A. Shinozaki, "Possibilities and limitations of Gaussian-closure approximations for phase-ordering dynamics," Phys. Rev. E **49** 2693–2699 (1994)

[11] C. Lubich, "On variational approximations in quantum molecular dynamics," Math. Comp. **74** 765–779 (2005)

[12] M. Benarous, "BEC from a time-dependent variational point of view," Ann. Phys. **320** 226–236 (2005)

Choose one (at least) of these papers and read it. Write a brief one- or two-page description of the paper, focussing particularly on the use of the Rayleigh-Ritz/PDF-closure method. Describe the *Ansatz* that the author(s) make for the solution of the problem, i.e. the quantum wavefunction or the distribution/density matrix & observables. What motivates this guess? How is the method implemented to obtain quantitative results? What are the principal conclusions of the paper?

Note that many of these papers are difficult (some *very* difficult). Don't worry if you don't understand every detail, but try to understand the main points.

If you find another paper applying the Rayleigh-Ritz/PDF-closure method to a research problem that is closer to your interests, send me a .pdf copy and, if suitable, you may discuss that paper instead.