Chapter 2

Moment Closures in One Dimension

To connect theory of kinetic fluid-moment closures to statistical closure theories, the main results of this chapter will be explained in terms of the stochastic oscillator problem (Kraichnan 1961; Kubo 1963; Kraichnan 1968), which is precisely analogous to the linearized Vlasov equation. Several common statistical closures are reviewed here, including simple truncation, cumulant discard, and Padé approximations.

One would like to evolve a finite set of equations for the first n statistical or fluid moments, denoted by $g_0(t), g_1(t), \ldots, g_{n-1}(t)$. The equation for $g_{n-1}(t)$ contains the next higher moment $g_n(t)$, which must somehow be approximated. Early simulations of the Vlasov equation (Armstrong et al. 1970) solved this problem by truncation [analogous to setting $g_n(t) = 0$] and noting that the simulations are only rigorously correct as long as the effect of the missing term is small. This time limit turns out to be a very severe restriction, however, since for a purely collisionless plasma the number of moments necessary to simulate a given time t is proportional to t^2. Even in highly collisionless plasma, though, one expects that the fluctuations transfered to finer and finer scales will eventually be wiped out by the small collisionality. It is reasonable, therefore, to propose a dissipative closure at a moderate number of moments that models the collisionless transfer to small scales. In fact, a closure of the form $g_n(t) = C_0 g_0(t) + \cdots + C_{n-1} g_{n-1}(t)$ was proposed by Knorr (1973) for series solutions of the Vlasov equation that guaranteed dissipative behavior. The size of the damping, which is determined by the coefficients, was left undetermined, however.

The linear response for the one-dimensional Vlasov equation is easily calculated and can be expressed in terms of the plasma dispersion function $Z(\zeta)$. Using the exact response, it is possible to construct a closed set of fluid equations that exactly reproduces the linear theory of the Vlasov equation (Chang and Callen 1992). Such a closure is frequency dependent, however, so implementation in numerical simulations would require the calculation of time-history integrals.

The novel idea of Hammett and Perkins (1990) was to construct linear single-time closures that have a very low computational cost. The resulting "Landau-fluid" equations are optimized to approximate the exact linear theory of the Vlasov equation by choosing appropriate closure coefficients. For n moment equations, matching in the "adiabatic" limit $\omega \to 0$ limit to $\mathcal{O}(\omega^q)$ and in the fluid limit $\omega \to \infty$ to $\mathcal{O}(\omega^{-(2n+1-q)})$, where $q \leq n$ is an integer, gives n conditions that uniquely determine all the coefficients. This procedure yields a set of equations with a linear response that matches the exact response somewhat uniformly over a wide range of frequencies. The choice of limits in which the matching is performed is somewhat arbitrary, but the limits $\omega \to \infty$ and $\omega \to 0$ are natural choices. Simply adding more moment equations improves the short-time response of the system and hence improves the matching in the high-frequency limit, $\omega \to \infty$. Matching purely in the high-frequency limit, however, yields a system of equations that fails to capture the long-time decay due to collisionless dissipation from Landau damping. Obtaining some conditions at low frequencies introduces dissipation into the closure that models Landau damping. (Hence, the Hammett–Perkins closure is often referred to as the Landau-fluid closure.) One might ask why the low-frequency matching is not performed at some other natural frequency, such as the mode frequency. The mode frequency for a given wavenumber is a complicated function of the background gradients and plasma parameters. Matching at $\omega \to 0$ yields simple expressions for the closure coefficients and gives a response that matches the exact response simultaneously at all frequencies. In the saturated turbulent state, fluctuations are not locked to the mode frequency, but instead are driven at over a broad band of frequencies by the nonlinear coupling to other modes. It is therefore appropriate to attempt to model the linear response simultaneously at all frequencies; the matching technique of Hammett–Perkins that is generalized here meets this objective.

In Section 2.7.1 it is demonstrated that for moment systems closed with this two-point closure the response function converges to the exact response function with increasing numbers of moments for the standard Gaussian (Maxwellian) background. Convergence is demonstrated for any fixed q, the number of times the response is matched in the $\omega \to 0$ limit, but the convergence is faster for larger q. Similar results were observed for three, four and five moment equations in the application of Landau-fluid closures to resistive g modes by Hedrick and Leboeuf (1992). Recently, a novel renormalization-group like approach to the Hermite series formulation was proposed by Parker and Carati (1995) to generate closures corresponding to the $q = 1$ case.

Orthogonal polynomial moments provide the natural basis for expressing results about linear closures for the stochastic oscillator and the Vlasov equation. The major results obtained in Section 2.6.1 concerning the behavior of the error of the approximate response function are expressed in terms of setting the first $n - q$ closure coefficients to 0. When the closure condition is not expressed in terms of orthogonal polynomials, the $n - q$ conditions for these results become general linear combinations of the closure coefficients with no simple form. The Vlasov equation is typically modeled by assuming a Maxwellian background. For a Maxwellian, the orthogonal moments are the Hermite moments defined in Section 3.3. The Hermite moments correspond precisely to the Hermite series expansions of the Vlasov equation considered in the past. It has often been observed for statistical closures that cumulants have nice properties (Kubo 1963). Cumulants are shown to be linearly equivalent to Hermite moments for linear closures about a Maxwellian background.

2.1 The Plasma Dispersion Function

The Laplace transform in time is a natural tool in the study of plasma instabilities, since the assumption of a fixed (in time) background distribution leads to differential equations with constant (in time) coefficients. The convention used here is to define the Laplace transform of a function of time, $f(t)$, by

$$\widehat{f}(\omega) = \int_0^\infty \exp(i\omega t) f(t)\, dt, \tag{2.1}$$

for ω with positive imaginary part, and by analytic continuation for ω in the lower-half complex plane. The inverse transform is given by

$$f(t) = \frac{1}{2\pi} \int_{-\infty+i\delta}^{\infty+i\delta} \exp(-i\omega t) \widehat{f}(\omega)\, d\omega, \tag{2.2}$$

where the $i\delta$ in the limits indicates that the contour is to be taken in the complex plane above any singularities of $\widehat{f}(\omega)$. At the risk of some ambiguity, the hats will be dropped throughout this thesis and $f(\omega)$ should be interpreted as the Laplace transform of $f(t)$.

Named by Fried and Conte (1961), the plasma dispersion function $Z(\zeta)$ can be written simply as the Laplace transform of a Gaussian time response:

$$Z(\zeta) = i \int_0^\infty \exp(i\zeta t) \exp(-t^2/4)\, dt. \tag{2.3}$$

The 'Z function' has the series and asymptotic expansions (Brook 1987)

$$Z(\zeta) \sim i \sum_{j=0}^{\infty} \frac{(2i)^j \Gamma((j+1)/2)}{\Gamma(j+1)} \zeta^j \qquad (\zeta \to 0), \tag{2.4}$$

$$Z(\zeta) \sim -\sum_{j=0}^{\infty} \frac{(2j)!}{j! 2^{2j}} \frac{1}{\zeta^{2j+1}} \qquad (|\zeta| \to \infty,\ \mathrm{Im}(\zeta) \geq 0). \tag{2.5}$$

Plotted for reference in Fig. 2.1, the Z function is useful for expressing the frequency response of systems involving Gaussian distributions.

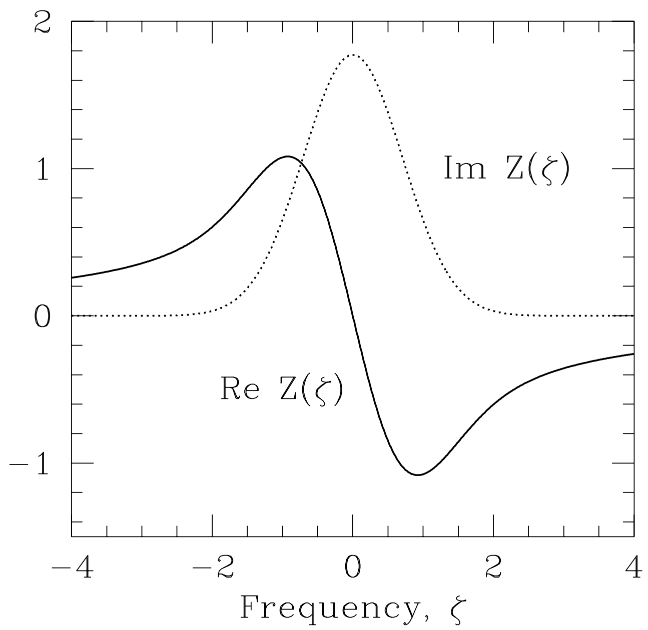

Figure 2.1: The plasma dispersion function.

2.2 The Stochastic Oscillator Problem

The random-oscillator problem is defined by the ensemble of initial-value problems,

$$\left(\frac{d}{dt}+\nu\right)y(t)+iby(t)=0, \qquad y(0)=1, \tag{2.6}$$

where b is a real-valued random variable with probability density function (PDF) $\rho(b)$. This oscillator equation has the simply computed exact solution

$$y(t)=\exp\bigl(-(ib+\nu)t\bigr) \qquad (t\geq 0), \tag{2.7}$$

and yet is sufficiently interesting to illustrate the behavior of several standard approximation schemes for turbulence (Kraichnan 1961). In the limit of no damping, $\nu\to 0$, the behavior of statistical moments of the oscillator equation is directly analogous to the behavior of fluid moments due to phase mixing.

A particular class of statistical moments is defined by

$$g_n(t)=\langle b^n y(t)\rangle\,, \tag{2.8}$$

where $\langle\cdot\rangle$ is an average over the ensemble of possible values of b. [The average can be written as $\langle f\rangle=\int_{-\infty}^{\infty} f\rho(b)\,db$.] One is typically interested in the time behavior of the lowest-order moments, $g_0(t)$ in particular. By taking moments of the oscillator solution (2.7), one directly obtains the exact time response

$$\begin{aligned} g_n(t) &= \langle b^n \exp(-(ib+\nu)t)\rangle \\ &= \int_{-\infty}^{\infty} b^n \exp(-(ib+\nu)t)\rho(b)\,db. \end{aligned} \tag{2.9}$$

The ensemble of amplitudes $y(t)$ have frequencies b with distribution $\rho(b)$. Initially $y(0) = 1$, so all realizations are "in-phase". As time progresses, the phases change at different frequencies and become decorrelated from one another. This *phase mixing* leads to a decay of the moments, since realizations that are out of phase ($\Delta bt \approx \pi$) will cancel one another. The spread in the frequencies (given by the standard deviation $\sqrt{\langle b^2\rangle - \langle b\rangle^2}$) is a good estimate of the rate of damping due to phase mixing. The dissipative closures introduced later in this chapter introduce a damping rate that scales with this frequency spread.

Several of the standard closure techniques will be applied to the case where b has a Gaussian distribution with PDF

$$\rho_G(b) = (2\pi)^{-1/2}\exp(-b^2/2). \tag{2.10}$$

In this case, the response of the lowest moment is just

$$g_0(t) = \exp(-t^2/2 - \nu t) \qquad (t \geq 0), \tag{2.11}$$

which is plotted against several approximation in Fig. 2.2. The decay is faster than exponential, so simple exponential damping at the same rate can only roughly model the true decay. However, as we will find, combining several moment equations with a dissipative closure of the right magnitude enables one capture both the short-time behavior $g_0(t) = 1 - \nu t + (\nu^2 - 1)t^2/2 + \cdots$ and the decay for large times.

2.3 Review of Closure Techniques

Taking moments of the oscillator equation (2.6) directly [operating on both sides by $\int_{-\infty}^{\infty} \cdot b^n \rho(b)\,db$], an infinite hierarchy of moment equations. The nth moment equation

$$\left(\frac{d}{dt} + \nu\right) g_n(t) + i g_{n+1}(t) = 0, \qquad g_n(0) = \langle b^n\rangle, \tag{2.12}$$

couples the nth moment to the $(n+1)$st moment. A finite subset of equations in this hierarchy cannot be solved directly, since the evolution of higher-order moments is required. A moment closure that expresses the nth moment $g_n(t)$ in terms of the first n moments $g_0(t), g_1(t), \ldots, g_{n-1}(t)$ can be used with the first n moment equations to form a closed finite system that approximates the infinite-dimensional moment system.

Definition 1
The n-moment system with closure for the stochastic oscillator problem is the system of equations

$$\begin{aligned}
\left(\frac{d}{dt}+\nu\right) g_0(t) &= -ig_1(t), & g_0(0) &= \langle 1 \rangle, \\
\left(\frac{d}{dt}+\nu\right) g_1(t) &= -ig_2(t), & g_1(0) &= \langle b \rangle, \\
&\vdots & &\vdots \\
\left(\frac{d}{dt}+\nu\right) g_{n-1}(t) &= -ig_n(t), & g_{n-1}(0) &= \left\langle b^{n-1} \right\rangle, \\
g_n(t) &= F(g_0, g_1, \ldots, g_{n-1}, t).
\end{aligned} \tag{2.13}$$

In general, the closure function $F(\cdot)$ can be nonlinear and can depend on the time histories of the resolved moments $g_0(t), g_1(t), \ldots, g_{n-1}(t)$. The solution of the closed moment system (2.13) will be denoted $g_0^{\mathrm{a}}(t), g_1^{\mathrm{a}}(t), \ldots, g_n^{\mathrm{a}}(t)$ in order to differentiate it from the exact solution (2.9).

A natural criterion for evaluating the performance of a given moment closure $F(\cdot)$ is the ability of the response $g_0^{\mathrm{a}}(t)$ for the lowest moment of the closed system to reproduce the exact response $g_0(t)$ from Eq. (2.9). For convergence of the two-point approximation closures considered in Section 2.7, the transformed approximate response $g_0^{\mathrm{a}}(\omega)$ will be compared to the transformed exact response $g_0(\omega)$.

The definition of a closure function used here is sufficiently general that one can trivially reproduce the exact response. When the frequencies have a Gaussian PDF, for example, the exact solution for the first moment is known, so the first moment closure

$$g_1(t) = F(g_0, t) \equiv -it\exp(-t^2/2 - \nu t) \tag{2.14}$$

and the zeroth moment equation form a system that exactly reproduces the response $g_0(t)$. This closure for the first moment uses no information about the state of the zeroth moment, and obviously leads to incorrect results for problems where the frequencies have a different non-Gaussian PDF (or even a Gaussian PDF with different variance). One would like to apply statistical closures to more complex problems, so the stochastic oscillator problem should be regarded as a simple test case only. In order to be generally applicable, a closure should be derived using as little information about the specific problem as is possible. The types of closure functions considered, the criterion used to evaluate convergence of a closure scheme, and the nature of convergence considered will all depend on the desired application.

For the statistical moment closure problem considered by Kraichnan (1968), the desired application of the closures is to statistical moment hierarchies arising in the study of fluid turbulence. For the statistical turbulence problem, the probability distributions of most field quantities are likely non-Gaussian, and one does not know ahead of time what form the probability distributions will take. In this case, it is unreasonable to use information about the probability distribution in the derivation of the closure. An expansion based on the form of the equations was derived by Kraichnan (1968). The result is a sequence of Padé approximations to the first moment of the form $g_1(\omega) = F_i(g_0(\omega))$, where $i \geq 0$ takes on integral values. (When this expression is transformed back to the time domain, it will contain time-history integrals when the function is nonlinear.)

The results obtained in this chapter will be applied to the derivation of fluid moment closures for the study of plasma instabilities. In contrast to the turbulence problem, the underlying distribution is assumed to be known. Information about the exact response will be used to construct linear closures for the nth moment of the form $g_n(t) = F_{n,q}(g_0(t), g_1(t), \ldots, g_{n-1}(t))$ for integers $0 < q \leq n < \infty$. The fluid moment closures are to be used in numerical simulations that follow the time evolution of plasma turbulence, so closures that involve time-history integrals are prohibitively expensive to compute. The linear closure function costs very little to compute, but has a limited number of degrees of freedom (n) that can be adjusted to fit the response. Convergence in this case is considered for a set of closures with increasing numbers of moments, $n \to \infty$, as opposed to the statistical turbulence closures that consider successively higher-order nonlinear closures for the first moment.

Note that the closure techniques derived in this chapter do not directly carry over to statistical moment closures for turbulence, since the form of the background distribution is used in deriving the closures. However, the nature of the convergence of the response for these linear closures with increasing numbers of moments may provide some insight for those attempting to extend nonlinear turbulence closures to arbitrary numbers of moments.

2.3.1 Realizability and the Approximate Distribution

An estimate for a finite set of statistical moments is called *realizable* if an ensemble of realizations with non-negative probability exists that has those moments (Kraichnan 1980). (By definition the true moments of a probability distribution are realizable.) Realizability constraints can lead to some interesting closures for turbulence models (Kraichnan 1985). For the problem at hand, the closed moment system (2.13), only single-time moments $\langle b^n y(t) \rangle$ that are first order in $y(t)$ are considered. A particular ensemble is constructed here that has a useful physical interpretation.

For the closed moment system (2.13) of the stochastic oscillator, it is possible to construct an ensemble of realizations that satisfy the stochastic oscillator evolution equation (2.6), but with a modified distribution of frequencies. From the exact solution (2.7) Kraichnan (1961) noted that, for $\nu = 0$, the PDF of b is related to the transform of the zeroth moment response by $\pi\rho(b) = \mathrm{Re}(g_0(\omega)|_{\omega=b})$. If the Laplace transform of an approximate solution $g_0^{\mathrm{a}}(t)$ exists for a given closed moment system, then we can define the *approximate distribution*

$$\rho^{\mathrm{a}}(b) = \frac{1}{\pi}\mathrm{Re}(\left. g_0^{\mathrm{a}}(\omega)\right|_{\omega=b}). \tag{2.15}$$

[The approximate distribution for a given closure is called the *spectral density* in the discussion by Kraichnan (1968).] The approximate distribution for an n-moment system with closure has the same moments to order n as the exact distribution $\rho(b)$. The one-time joint PDF for b and $y(t) = y_r + iy_i$ given by

$$P(b, y_r, y_i) = \rho^{\mathrm{a}}(b)\delta(y_r - \cos(bt))\delta(y_i + \sin(bt)) \tag{2.16}$$

describes an ensemble of realizations with moments that satisfy the closed moment system (2.13). A requirement that the approximate distribution be non-negative, $\rho^{\mathrm{a}}(b) \geq 0$, can be viewed as a kind of realizability condition. (A closed moment system may yield an approximate distribution that fails this criterion and still be realizable, however.)

In the analogy between the stochastic oscillator problem and the linearized Vlasov equation, the PDF $\rho(b)$ corresponds to the background distribution. For a given fluid approximation, Hammett and Perkins (1990) define the *equivalent background distribution* f_0 in a manner analogous to the definition of the approximate distribution here. Requiring that the background distribution be non-negative leads to the condition on the approximate distribution, $\rho^{\mathrm{a}}(b) \geq 0$. (This condition is desirable even if one has no philosophical qualms with a negative distribution of particles. A background distribution of particles that goes negative for some velocities can lead to spurious bump-on-tail instabilities.)

2.3.2 Taylor-Series Approximation

The simplest possible closure for the n-moment system (2.13) would evolve the first n equations and set the nth moment to zero, $g_n(t) = 0$, where it arises in the $(n-1)$st equation. [The closure function is simply $F(g_0, \ldots, g_{n-1}) = 0$.] The solution of the truncated system,

$$g_0^{\mathrm{a}}(t) = \sum_{j=0}^{n-1}(-i)^j \left\langle b^j \right\rangle \frac{t^j}{j!}, \tag{2.17}$$

is a Taylor-series approximation to the true response (2.9). This series converges to the correct answer for any fixed time t as $n \to \infty$. For a fixed number of moment equations, however, the approximate solution behaves horribly for large t, blowing up instead of decaying to zero. The truncated system has no approximate distribution, since the Laplace transform of the response does not exist.

2.3.3 Cumulant-Discard Approximation

Another commonly used approximation scheme is found by assuming that the nth cumulant average is zero, $\langle b^n y(t)\rangle_c = 0$. Cumulant averages for two variables b and y are defined by identifying coefficients of powers of λ and γ in the series expansion of the equation

$$\langle \exp(\lambda b + \gamma y)\rangle = \exp\left(\sum_{j+k\geq 1}^{\infty} \frac{\lambda^j}{j!}\frac{\gamma^k}{k!} \left\langle b^j y^k \right\rangle_c \right) \tag{2.18}$$

(Kubo 1963). One is interested in moments and cumulants that are first order in y such as $g_n = \langle b^n y\rangle$. The first derivative of the cumulant definition (2.18) with respect to γ evaluated at $\gamma = 0$ is the expression

$$\langle y \exp(\lambda b)\rangle = \left(\sum_{j=0}^{\infty} \frac{\lambda^j}{j!} \left\langle b^j y \right\rangle_c \right) \exp\left(\sum_{j=1}^{\infty} \frac{\lambda^j}{j!} \left\langle b^j \right\rangle_c \right), \tag{2.19}$$

which relates the moments and cumulants that are first order in y. Using this definition, one can obtain closure approximations for an arbitrary number of moments,

$$\begin{aligned}
g_1(t) =& \langle b\rangle\, g_0(t),\\
g_2(t) =& 2\langle b\rangle\, g_1(t) + \left(\left\langle b^2\right\rangle - 2\langle b\rangle^2\right) g_0(t),\\
g_3(t) =& 3\langle b\rangle\, g_2(t) + \left(3\left\langle b^2\right\rangle - 6\langle b\rangle^2\right) g_1(t) + \left(\left\langle b^3\right\rangle - 6\left\langle b^2\right\rangle\langle b\rangle + 6\langle b\rangle^3\right) g_0(t),\\
g_4(t) =& 4\langle b\rangle\, g_3(t) + \left(6\left\langle b^2\right\rangle - 12\langle b\rangle^2\right) g_2(t) + \left(4\left\langle b^3\right\rangle - 24\left\langle b^2\right\rangle\langle b\rangle + 24\langle b\rangle^3\right) g_1(t),\\
&+ \left(\left\langle b^4\right\rangle - 8\left\langle b^3\right\rangle\langle b\rangle + 36\left\langle b^2\right\rangle\langle b\rangle^2 - 6\left\langle b^2\right\rangle^2 - 24\langle b\rangle^4\right) g_0(t),\\
&\vdots
\end{aligned} \tag{2.20}$$

For centered Gaussian distributions, the only nonzero cumulant is the second-order cumulant, so cumulant expansions work very well when the actual PDF is nearly Gaussian. Kraichnan (1961) illustrated the behavior of the cumulant discard closure on the stochastic oscillator problem by considering the fourth-cumulant closure, which takes the form

$$g_4(t) = 6g_2(t) - 3g_0(t), \tag{2.21}$$

when the frequency b has a Gaussian distribution (2.10). For the closed system containing this closure and the first three moment equations (2.12), the lowest moment evolves as

$$g_0^{\mathrm{a}}(t) = \frac{1}{6}\left[(3-\sqrt{6})\cos(t\sqrt{3+\sqrt{6}}) + (3+\sqrt{6})\cos(t\sqrt{3-\sqrt{6}})\right]. \tag{2.22}$$

Unlike the simple closure that yields a power series, this approximation gives a solution that at least remains bounded for $t \to \infty$. Also, the error from the exact solution (2.11) as $t \to 0$ is $\mathcal{O}(t^8)$ for the fourth-cumulant closure instead of the $\mathcal{O}(t^4)$ error that one obtains from the simple fourth moment closure $g_4(t) = 0$. This closed system has a non-negative approximate distribution that can be written as the sum of delta functions,

$$\begin{aligned}\rho^{\mathrm{a}}(b) = &\frac{3-\sqrt{6}}{12}\left[\delta(b-\sqrt{3+\sqrt{6}})+\delta(b+\sqrt{3+\sqrt{6}})\right] \\ &+\frac{3+\sqrt{6}}{12}\left[\delta(b-\sqrt{3-\sqrt{6}})+\delta(b+\sqrt{3-\sqrt{6}})\right],\end{aligned} \tag{2.23}$$

which is quite unlike the true continuous Gaussian distribution.

Several results of the cumulant closure approach in the aforementioned case—realizability, bounded solutions, and higher-order accuracy as $t \to 0$—arise because a Gaussian distribution of frequencies was assumed. For a Gaussian distribution (2.10) of frequencies, the first-order cumulant equation (2.19) becomes

$$\begin{aligned}\sum_{j=0}^{\infty}\frac{\lambda^j}{j!}\left\langle b^j y\right\rangle_c &= \langle y\exp(\lambda b)\rangle\exp(-\lambda^2/2) \\ &= \left\langle y\exp(2(\lambda/\sqrt{2})(b/\sqrt{2})-(\lambda/\sqrt{2})^2)\right\rangle \\ &= \sum_{j=0}^{\infty}\frac{\lambda^j}{j!}2^{-j/2}\left\langle H_j(b/\sqrt{2})y\right\rangle,\end{aligned} \tag{2.24}$$

where H_j is the jth Hermite polynomial defined in Table 2.1. (The exponential generating function for Hermite polynomials,

$$\exp(2xt-t^2) = \sum_{j=0}^{\infty}\frac{t^j}{j!}H_j(x), \tag{2.25}$$

is used to obtain this result.) Therefore, the cumulant averages can be written as

$$\langle b^n y\rangle_c = 2^{-n/2}\left\langle H_n(b/\sqrt{2})y\right\rangle. \tag{2.26}$$

The Hermite polynomials $H_n(x/\sqrt{2})$ are also the orthogonal polynomials with respect to the weight function given by the Gaussian distribution. For a Gaussian distribution, therefore, the nth cumulant-discard closure is equivalent to setting the nth orthogonal-polynomial moment to zero. Realizability and bounded solutions for systems closed by truncation in orthogonal-polynomial moments follows from the connection to the physical mass–spring system demonstrated in Section 2.7.2. The higher-order accuracy as $t \to 0$ for orthogonal polynomial moment truncation is a simple corollary of the asymptotic behavior of this form of closure demonstrated in

Result 4. However, note that for non-Gaussian distributions the cumulant moments will be different in general from the orthogonal polynomial moments. Thus, the cumulant-discard approach should not be expected to produce bounded solutions in general.

One can easily construct examples where the cumulant-discard procedure fails. Consider a distribution with large kurtosis ($\langle b^4\rangle/\langle b^2\rangle^2$),

$$\rho(b) = \frac{1}{187\sqrt{2\pi}}\left[\frac{81}{7}\exp(-9x^2/98) + 320\exp(-2x^2)\right], \tag{2.27}$$

which has moments, $\langle b\rangle = 0$, $\langle b^2\rangle = 1$, $\langle b^3\rangle = 0$, $\langle b^4\rangle = 13$, and so on. Using the fourth-cumulant closure for this example [$g_4(t) = 6g_2(t) + 7g_0(t)$ in this case] gives the approximate response

$$g_0^{\mathrm{a}}(t) = \frac{1}{4}\cos(\sqrt{7}t) + \frac{3}{4}\cosh(t). \tag{2.28}$$

The approximation in this case blows up exponentially as $t \to \infty$, and only matches the true solution as $t \to 0$ to $\mathcal{O}(t^4)$.

2.3.4 Padé Approximations

Padé approximation refers to the use of ratios of polynomials to approximate functions. They are a standard tool in analysis that can often give uniformly excellent approximations to functions even in situations where series approximations are divergent. The monographs of Baker (1975) and Baker and Graves-Morris (1996) provide an excellent overview of Padé theory and are the source of the basic results and notation used in this thesis.

Definition 2
Suppose a function $f(z)$ has a power series $f(z) = c_0 + c_1 z + c_2 z^2 + \cdots$. The L, M Padé Approximant *to f is a ratio of polynomials*

$$[L/M]_f(z) = \frac{Q^{[L/M]}(z)}{P^{[L/M]}(z)} \tag{2.29}$$

such that $Q^{[L/M]}(z)$ is a polynomial of degree at most L, $P^{[L/M]}(z)$ is a polynomial of degree at most M, and the first $L+M+1$ coefficients in the series for $[L/M] - f(z)$ are zero. Padé approximants to an asymptotic series $f(w) = c_0 + c_1 w^{-1} + c_2 w^{-2} + \cdots$ are obtained by taking $z = 1/w$ in the defining equation (2.29).

One expects to be able to fulfill the $L+M+1$ conditions required to match the series since $Q^{[L/M]}(z)$ has $L+1$ coefficients, $P^{[L/M]}(z)$ has $M+1$ coefficients, and one degree of freedom is lost since the ratio is taken. It is possible with this definition for the Padé approximation to fail to exist in some cases.

Kraichnan (1968) obtains interesting Padé approximations to the response function by considering the Laplace transform of the moment equations (2.12),

$$
\begin{aligned}
(-i\omega+\nu)g_0(\omega)+ig_1(\omega) &= 1, \\
(-i\omega+\nu)g_1(\omega)+ig_2(\omega) &= \langle b\rangle, \\
(-i\omega+\nu)g_2(\omega)+ig_3(\omega) &= \left\langle b^2\right\rangle, \\
&\vdots
\end{aligned}
\tag{2.30}
$$

Upon expanding in inverse powers of $\omega+i\nu$, one easily obtains the asymptotic series solution

$$
g_0(\omega)=i\sum_{j=0}^{\infty}\frac{\langle b^j\rangle}{(\omega+i\nu)^{j+1}}, \tag{2.31}
$$

which can be divergent for distributions of interest.

For example, consider the Gaussian case with the distribution in Eq. (2.10). The exact response is

$$
g_0(\omega)=-iZ((\omega+i\nu)/\sqrt{2})/\sqrt{2}, \tag{2.32}
$$

and the asymptotic series (2.31) is divergent for all choices of ω and ν in this case. The N,N Padé approximations to g_0,

$$
\begin{aligned}
[1/1]_g(\omega) &= i\frac{(\omega+i\nu)^{-1}}{1}, \\
[2/2]_g(\omega) &= i\frac{(\omega+i\nu)^{-1}}{1-(\omega+i\nu)^{-2}}, \\
[3/3]_g(\omega) &= i\frac{(\omega+i\nu)^{-1}-(\omega+i\nu)^{-3}}{1-3(\omega+i\nu)^{-2}}, \\
&\vdots
\end{aligned}
\tag{2.33}
$$

are equivalent to the solutions obtained using the cumulant-discard closure (2.20) for the Nth moment. The diagonal Padé series $[0/0], [1/1], [2/2], \ldots$ corresponds to convergents of a Jacobi-type continued fraction. In this case the continued fraction expansion

$$
g_0(\omega)=\cfrac{i}{\omega+i\nu-\cfrac{1}{\omega+i\nu-\cfrac{2}{\omega+i\nu-\cfrac{3}{\omega+i\nu-\cdots}}}} \tag{2.34}
$$

converges for $\nu > 0$, but diverges for $\nu = 0$ (Kraichnan 1968; Wall 1967). The Padé series is therefore an improvement over the asymptotic series. Many physical problems of interest, however, are analogous to the low-dissipation limit $\nu \to 0$, where even the Padé series converges increasingly poorly.

The Padé and asymptotic series are derived in the high-frequency $\omega \to \infty$ limit. This limit is matched naturally for the closed moment system (2.13) as increasing numbers of moments are taken. The cumulant discard approximation and the Padé approximation discussed here match the exact response extremely well in the high-frequency limit, but fail to capture the long-time decay due to phase mixing. The Landau-fluid closures achieve highly accurate response functions by generalizing to two-point Padé approximations that are constructed by matching in the low-frequency limit $\omega \to 0$ as well as the high-frequency limit $\omega \to \infty$.

2.3.5 Random-Coupling Model

An alternate approach suggested by Kraichnan (1968) is to consider expansion in powers of the response $g_0(\omega)$ itself. For the Gaussian case, there is evidence that the continued fraction expansion

$$ig_1(\omega) = \cfrac{g_0(\omega)^2}{1 + \cfrac{g_0(\omega)^2}{1 + \cfrac{3g_0(\omega)^2}{1 + \cfrac{11g_0(\omega)^2}{1 + \cdots}}}} \tag{2.35}$$

converges even in the limit $\nu = 0$, and therefore provides more robust closure approximations. The lowest-order approximation,

$$ig_1(\omega) = g_0(\omega)^2, \tag{2.36}$$

is equivalent to the random-coupling approximation of Kraichnan (1961). This closure has a corresponding non-negative approximate distribution

$$\rho^{\mathrm{a}}(b) = \frac{1}{\pi}\sqrt{1 - (b/2)^2} \qquad (-2 \leq b \leq 2), \tag{2.37}$$

and gives the time response

$$g_0(t) = J_1(2t)/t, \tag{2.38}$$

where J_n denotes the standard Bessel function of the first kind. One obtains a response that decays to zero as $t \to \infty$ with this approximation at the expense of introducing a nonlinear closure.

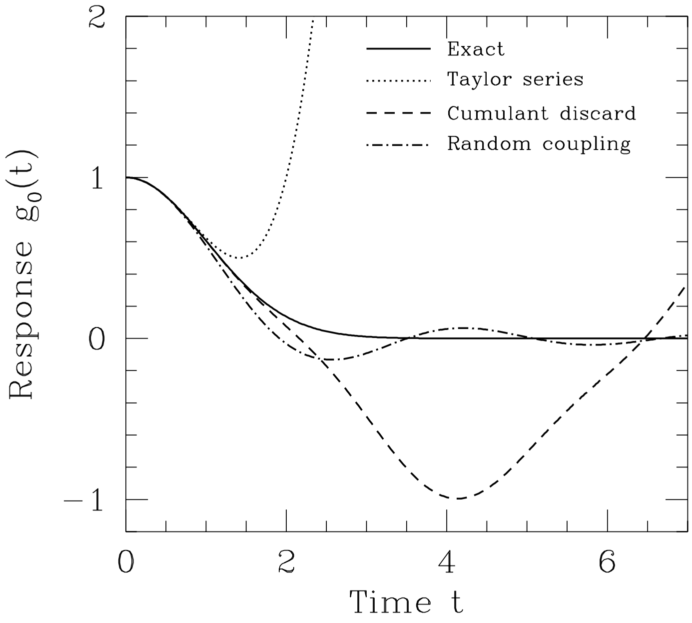

Figure 2.2: Response functions obtained from several approximation schemes for the stochastic oscillator with Gaussian-distributed b and $\nu = 0$. Results are displayed for the fourth-order Taylor-series approximation (2.17), the fourth-cumulant discard closure (2.21), and the random-coupling approximation (2.36). The random-coupling approximation matches the exact response to $\mathcal{O}(t^3)$ as $t \to 0$.

2.3.6 Hammett–Perkins Closure

Consider a generalization of the cumulant-discard closure to a linear closure with arbitrary coefficients. The simplest such closure is the a linear closure for the first moment,

$$g_1(\omega) = A_0 g_0(\omega). \tag{2.39}$$

[For constant A_0, the closure is the same in the time domain; $g_1(t) = A_0 g_0(t)$.] In reality, the first moment $g_1(\omega)$ is not simply a multiple of $g_0(\omega)$, so this closure cannot be exact. The advantage to constant linear closures of this form is that they are easily implemented in numerical simulations. [Replacing A_0 with $\omega + \sqrt{2}/Z(\omega/\sqrt{2})$ in Eq. (2.39) results in a closure that matches the response exactly. However, implementing such a closure in a numerical simulation would require expensive computations of time-history integrals.] Using the Laplace transformed stochastic oscillator

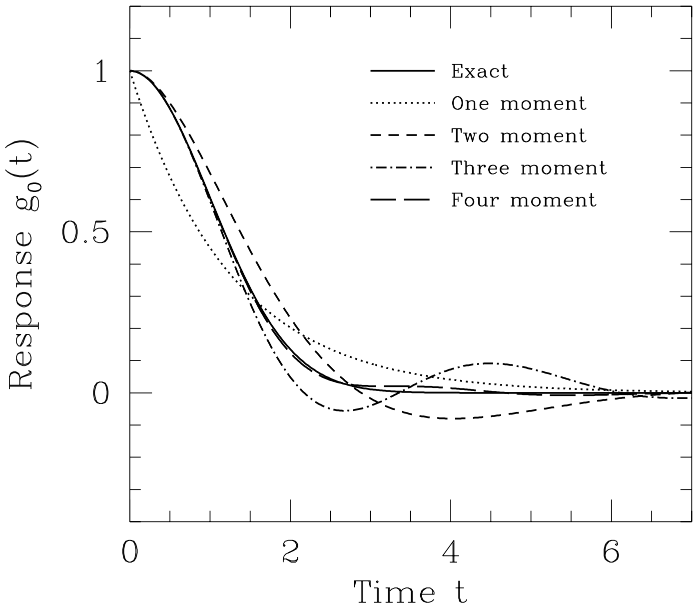

Figure 2.3: Response functions obtained using one, two, three, and four moment Hammett–Perkins closures compared to the exact time response for the stochastic oscillator with Gaussian-distributed b and $\nu = 0$.

equations (2.31) in the limit $\nu = 0$, one easily finds the response for this closure,

$$g_0^{\mathrm{a}}(\omega) = i\frac{1}{\omega - A_0}. \tag{2.40}$$

We would like to choose the closure coefficient A_0 so that this approximate response is a good estimate of the exact response (2.32). Hammett and Perkins (1990) considered linear closures of this form where the coefficients are chosen by matching the exact response in the $\omega = 0$ limit as well as $\omega \to \infty$. (The structure of moment equations causes the response to match in the high-frequency limit as more moment equations are added, and the low-frequency limit gives conditions that cause the coefficients to capture the physics of Landau damping.) The resulting closures yield linear responses that match the exact response well simultaneously at all frequencies. For the first moment closure here, taking $A_0 = -i\sqrt{2/\pi}$ matches the exact response (2.32) at $\omega = 0$. [Alternately, one could derive this closure by considering the low frequency limit of the exact closure coefficient $\omega + \sqrt{2}/Z(\omega/\sqrt{2})$.]

To illustrate the method more generally, consider the fourth-moment closure

$$g_4(\omega) = A_3 g_3(\omega) + A_2 g_2(\omega) + A_1 g_1(\omega) + A_0 g_0(\omega). \tag{2.41}$$

For the Gaussian case with $\nu = 0$, this closure results in a Padé approximation to the exact response,

$$g_0^{\mathrm{a}}(\omega) = i\frac{\omega^3 + \omega - A_3(\omega^2+1) - A_2\omega - A_1}{\omega^4 - A_3\omega^3 - A_2\omega^2 - A_1\omega - A_0}. \tag{2.42}$$

The coefficients (A_0, A_1, A_2, A_3) can now be chosen to try to approximate the true response (2.32). Matching the asymptotic series (2.31) to $\mathcal{O}(\omega^{-8})$ gives conditions on the coefficients that yields $A_0 = -3, A_1 = 0, A_2 = 6, A_3 = 0$, which is just the fourth-cumulant closure (2.21). [Note that the form of Eq. (2.42) already matches the asymptotic series to $\mathcal{O}(\omega^{-4})$ for any choice of coefficients, so matching to $\mathcal{O}(\omega^{-8})$ gives four conditions.] If one obtains two conditions by matching the response to $\mathcal{O}(\omega^6)$ at $\omega \to \infty$ and two conditions from matching to $\mathcal{O}(\omega)$ at $\omega = 0$, one finds the closure approximation

$$g_4(\omega) = (6+2\beta_1)g_2(\omega) - (3+2\beta_1)g_0(\omega) - \sqrt{2}D_1 i\left[g_3(\omega) - 3g_1(\omega)\right], \tag{2.43}$$

where $D_1 = 2\sqrt{\pi}/(3\pi - 8)$ and $\beta_1 = (32 - 9\pi)/(6\pi - 16)$, which corresponds to the four-moment Landau-fluid closure. This closure has a non-negative approximate distribution and the time response is almost indistinguishable from the exact response. (See Fig. 2.3.) The approximate response

$$g_0^{\mathrm{a}}(\omega) = \cfrac{i}{\omega - \cfrac{1}{\omega - \cfrac{2}{\omega - \cfrac{3+2\beta_1}{\omega + i\sqrt{2}D_1}}}} \tag{2.44}$$

is obtained using this closure, and is written here in continued fraction form for comparison with the expansion (2.34). The Hammett–Perkins closures for one, two, three, and four moments are plotted in Fig. 2.3.

One should note that there are some philosophical differences between the Hammett-Perkins Landau-fluid closure approach and the Kraichnan random-coupling approximation. The higher order Landau-fluid models fit the exact response somewhat better, particularly in the long-time decay where the random-coupling model has only an algebraic decay. In part, the improved fit arises because the derivation of the Landau-fluid approximation uses information known about the exact solution. The random-coupling model was derived without reference to the exact response, and is intended for more complicated problems where the distribution is most likely not Gaussian. While the Landau-fluid closure coefficients were chosen by fitting an idealized problem where the exact solution is know, it also is intended for use in more complicated problems where the exact solution is no longer known [such as happens when $\mathbf{E}\times\mathbf{B}$ nonlinearities are added to the Vlasov Eq. (3.5)]. The Landau-fluid closure is intended to model a subset of the physics known to reside in the more complicated problems. As we will find, the Hammett-Perkins closure works not only if the underlying distribution function is Gaussian, but it works in more general cases where the distribution function is sufficiently smooth that it can be written as a Gaussian times a few low order Hermite polynomials (no more than the number of moments being used).

2.4 Orthogonal Polynomials

The stochastic variable $y(t)$ is a continuous function of the frequency variable b and cannot therefore be fully characterized by a finite set of moments. Moment closure schemes attempt in some sense to estimate the effects of the missing or unresolved information. There are several interesting questions that one might ask. How does one estimate the PDF, given a finite set of moments? Is there a sensible definition of the 'unresolved scales' for this problem? What is a good estimate for the unresolved scales, given the observed moments? Note that answers to these questions can provide useful moment closure schemes. However, as was seen in the previous section, closures can be produced to fit the response functions without addressing any of these questions.

Expansions in orthogonal polynomials provide a natural translation from moments to underlying functions expressing those moments. Kraichnan (1970) noted that orthogonal polynomial expansions can be used to generate robust convergents to spectral densities given moments. Several results concerning linear closures for moment equations are readily expressed in terms of orthogonal polynomials.

2.4.1 Definition

Orthogonal polynomials are defined with respect to a positive weight function $w(x)$ for which the moments,

$$m_n = \int_{-\infty}^{\infty} x^n w(x)\, dx, \tag{2.45}$$

exist. It will be assumed that $m_0 = 1$ since $w(x)$ has the meaning of a probability density function. [The weight function $w(x)$ must decay faster than algebraically as $|x| \to \infty$ for all the moments to exist.]

Definition 3
Orthonormal polynomials with respect to a given weight function $w(x)$ are defined to be the polynomials in x,

$$P_n(x) = P_{n,0} + P_{n,1}x + P_{n,2}x^2 + \cdots + P_{n,n}x^n, \tag{2.46}$$

Polynomial	Definition	a_n	b_n	c_n
Hermite	$H_n(x) = (-1)^n \exp(x^2) \frac{d^n}{dx^n} \exp(-x^2)$	2	0	$2(n-1)$
Chebyshev	$U_n(x) = \frac{\sin((n+1)\arccos(x))}{\sin(\arccos(x))}$	2	0	1
Legendre	$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n}(x^2-1)^n$	$\frac{2n-1}{n}$	0	$\frac{n-1}{n}$
Laguerre	$L_n(x) = \frac{1}{n!} \exp(x) \frac{d^n}{dx^n} \exp(-x)$	$-\frac{1}{n}$	$\frac{2n-1}{n}$	$\frac{n-1}{n}$

Table 2.1: Definitions of commonly used orthogonal polynomials and recursion coefficients such that $P_n(x) = (a_n x + b_n)P_{n-1}(x) - c_n P_{n-2}(x)$. Notation and normalizations are taken from Gradshteyn and Ryzhik (1980).

that satisfy the orthogonality conditions

$$\int_{-\infty}^{\infty} P_n(x) P_m(x) w(x)\, dx = \delta_{nm}. \tag{2.47}$$

(The Kronecker delta function is defined by $\delta_{nm} = 1$ if $n = m$ and $\delta_{nm} = 0$ otherwise.)

Orthonormal polynomials can be shown to satisfy a three-term recurrence relation,

$$P_n(x) = (a_n x + b_n)\, P_{n-1}(x) - c_n P_{n-2}(x). \tag{2.48}$$

The recurrence coefficients are related to the leading coefficients of the polynomials through

$$a_n = \frac{P_{n,n}}{P_{n-1,n-1}}, \quad b_n = a_n \left(\frac{P_{n,n-1}}{P_{n,n}} - \frac{P_{n-1,n-2}}{P_{n-1,n-1}} \right), \quad c_n = \frac{a_n}{a_{n-1}}. \tag{2.49}$$

2.4.2 Orthogonal Polynomial Expansion

Orthogonal polynomial moments of an arbitrary function $f(x)$ are defined by

$$f_n = \int_{-\infty}^{\infty} P_n(x) f(x)\, dx. \tag{2.50}$$

The inverse transform from moments to the function $f(x)$ is defined formally by

$$f(x) = \sum_{j=0}^{\infty} f_j P_j(x) w(x). \tag{2.51}$$

weight $w(b)$		polynomial
Gaussian	$w_G(b) = \frac{1}{\sqrt{2\pi}} \exp(-b^2/2)$	$\frac{1}{\sqrt{n!2^n}} H_n(b/\sqrt{2})$
Spring	$w_s(b) = \begin{cases} \frac{1}{\pi}\sqrt{1-(b/2)^2} & (\lvert b\rvert < 2), \\ 0 & (\lvert b\rvert \geq 2) \end{cases}$	$U_n(b/2)$
Water Bag	$w_w(b) = \begin{cases} 1/2 & (\lvert b\rvert < 1), \\ 0 & (\lvert b\rvert \geq 1) \end{cases}$	$\sqrt{2n+1}P_n(b)$
Exponential	$w_e(b) = \begin{cases} \exp(-b) & (b > 0), \\ 0 & (b < 0) \end{cases}$	$L_n(b)$

Table 2.2: Orthonormal polynomials for weights corresponding to some PDFs of interest.

The form of these transforms is slightly asymmetric because one is expanding underlying distributions that decay rapidly for $|x| \to \infty$ in terms of moments that are polynomials, which diverge for large x. The weight function $w(x)$ appears in the moment expansion (2.51) to give the basic form of the modeled distributions.

It is possible to find functions whose orthogonal moment expansions do not converge pointwise or have poor pointwise convergence. Discontinuous functions, for example, will exhibit the ringing phenomenon observed in Fourier series expansions around discontinuities. The moment expansion does converge in an appropriately defined Hilbert space, however. The inner product

$$\langle f, g \rangle_w = \int_{-\infty}^{\infty} f(x)g(x)w(x)^{-1}\, dx \tag{2.52}$$

and corresponding norm $\|\cdot\|_w$ define a Hilbert space of distribution functions $\mathcal{H}_w$. If the set of functions $E_n = P_n(x)w(x)$ form a complete basis for $\mathcal{H}_w$, then the Fourier series

$$f = \sum_{j=0}^{\infty} \langle E_n, f \rangle_w\, E_n \tag{2.53}$$

converges for all $f \in \mathcal{H}_w$ [Theorem 4.13 of Conway (1990)]. Kraichnan (1970) demonstrates completeness for a broad class of $w(x)$. The moment expansion (2.51) can therefore be viewed as an orthonormal series expansion in $\mathcal{H}_w$, since from Eqs. (2.50) and (2.52) the expansion coefficients are given by $f_n = \langle E_n, f \rangle_w$.

2.5 Orthogonal Moments of the Stochastic Oscillator

The closure problem for stochastic oscillator moments is best studied in terms of polynomial moments, where the polynomials are *orthogonal with respect to the underlying PDF*. The main advantage to this orthogonal-polynomial expansion is demonstrated in Result 4, where it will be shown that matching in the high-frequency limit is simply accomplished by setting closure coefficients to zero. As well, projection onto orthogonal functions preserves the anti-Hermitian nature of the operator ib, so simple truncation at least gives solutions that are bounded in time.

Consider now the stochastic oscillator problem with underlying distribution written as an orthogonal-polynomial expansion about some positive weight function $w(b)$,

$$\rho(b) = \sum_{j=0}^{m} C_j P_j(b) w(b). \tag{2.54}$$

[This general form of the problem is useful when the results are carried over to the fluid moment problem where the initial conditions are of a form $\propto v f_M(v)$, which is a polynomial multiplied by a positive density function.] The *orthogonal-polynomial moments* are defined by

$$\alpha_n(t) = \langle P_n(b) y(t) \rangle , \tag{2.55}$$

where $P_n(b)$ are taken to be the orthonormal polynomials with respect to the same weight function $w(b)$. The general linear closure for the nth orthogonal-polynomial moment is then written as

$$\alpha_n(t) = \sum_{j=0}^{n-1} A_j \alpha_j(t). \tag{2.56}$$

2.5.1 Equivalence to b^n Moments

The first n polynomial moments $\{\alpha_0(t), \ldots, \alpha_{n-1}(t)\}$ contain exactly the same information as the first n moments $\{g_0(t), \ldots, g_{n-1}(t)\}$, so the resulting linear systems are equivalent. The translation from the problem with b^n moments $g_i(t)$, underlying distribution $\rho(b) = \sum_{j=0}^{m} C'_j b^j w(b)$ and closure $g_n(t) = \sum_{j=0}^{n-1} A'_j g_j(t)$ to the problem with polynomial moments (2.55), distribution (2.54), and closure (2.56) can be accomplished through

$$\begin{bmatrix} \alpha_0(t) \\ \alpha_1(t) \\ \vdots \\ \alpha_{n-1}(t) \end{bmatrix} = \mathsf{D}_{n-1} \begin{bmatrix} g_0(t) \\ g_1(t) \\ \vdots \\ g_{n-1}(t) \end{bmatrix}, \tag{2.57}$$

$$\begin{bmatrix} C_0 & C_1 & \dots & C_m \end{bmatrix} = \begin{bmatrix} C'_0 & C'_1 & \dots & C'_m \end{bmatrix} \mathsf{D}_m^{-1}, \tag{2.58}$$

$$\begin{bmatrix} A_0 & A_1 & \dots & A_n & -1 \end{bmatrix} = d_{nn} \begin{bmatrix} A'_0 & A'_1 & \dots & A'_{n-1} & -1 \end{bmatrix} \mathsf{D}_n^{-1}, \tag{2.59}$$

where the matrix of coefficients D is defined by

$$\mathsf{D}_k = \begin{bmatrix} P_{0,0} & 0 & \dots & 0 \\ P_{1,0} & P_{1,1} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ P_{k,0} & P_{k,1} & \dots & P_{k,k} \end{bmatrix}. \tag{2.60}$$

2.5.2 Exact Solution

Upon taking orthogonal-polynomial moments of the exact solution (2.7) in the limit $\nu = 0$, one obtains the general response

$$\alpha_k(t) = \sum_{j=0}^{m} \mathsf{R}_{kj}(t) C_j, \tag{2.61}$$

$$\mathsf{R}_{kj}(t) = \int_{-\infty}^{\infty} e^{-ibt} P_k(b) P_j(b) w(b)\, db. \tag{2.62}$$

The first result obtained here shows that the general element of the transformed response matrix

$$\mathsf{R}_{kj}(\omega) = \int_0^{\infty} e^{i\omega t} \int_{-\infty}^{\infty} e^{-ibt} P_k(b) P_j(b) w(b)\, db\, dt \tag{2.63}$$

can be expressed in terms of the basic response element $\mathsf{R}_{00}(\omega)$, the orthogonal polynomials $P_n(\omega)$, and a set of numerator polynomials $Q_n(\omega)$ defined here.

Definition 4
Given an orthonormal set of polynomials $P_n(x)$ satisfying the recurrence relation (2.48), the conjugate *or* numerator *polynomials $Q_n(x)$ are defined to be the set of polynomials satisfying the same recurrence relation (2.48), with $Q_0(x) = 0$ and $Q_1(x) = a_1$.*

Note that the polynomial $Q_n(x)$ has degree $n-1$, whereas $P_n(x)$ has degree n. It is easily shown that

$$P_{n-1}(x) Q_n(x) - P_n(x) Q_{n-1}(x) = a_n. \tag{2.64}$$

This identity is easily proved using induction, the recurrence relation (2.48), and the fact $c_n a_{n-1} = a_n$, which follows from orthonormality. In general there is no guarantee that the conjugate polynomials Q_n corresponding to common orthogonal polynomials can be expressed simply. Two exceptions worth mentioning are the Chebyshev polynomials $U_n(x)$, for which $Q_n(x) = U_{n-1}(x)/2$, and the Hermite polynomials, which can be defined along with their conjugates by

$$(d/d\zeta)^n Z(\zeta) = H_n(\zeta)Z(\zeta) + Q_n(\zeta). \tag{2.65}$$

Lemma 1
The response function $\mathsf{R}_{0j}(t)$ has a Taylor series at $t = 0$ whose first j coefficients vanish. In other words,

$$\mathsf{R}_{0j}(t) = 0 + 0t + \cdots + 0t^{j-1} + c_j t^j + \cdots . \tag{2.66}$$

Proof. Upon evaluating the kth derivative of the response (2.62), one finds that

$$\begin{aligned} \left|(\partial/\partial t)^k \mathsf{R}_{0j}(t)\right|_{t\,=\,0} &= \left|(\partial/\partial t)^k \int_{-\infty}^{\infty} e^{-ibt} P_j(b)w(b)\,db\right|_{t\,=\,0} \\ &= (-i)^k \int_{-\infty}^{\infty} b^k P_j(b)w(b)\,db. \end{aligned} \tag{2.67}$$

By definition, $P_j(b)$ is orthogonal to a complete set of polynomials with degree less than j, so the right-hand side of Eq. (2.67) is zero if $k < j$. $\square$

An immediate corollary to this is that the first term in the asymptotic series of the frequency response $\mathsf{R}_{0j}(\omega)$ is $\mathcal{O}(\omega^{-j-1})$. In other words,

$$\mathsf{R}_{0j}(\omega) \sim i\frac{i^j j! c_j}{\omega^{j+1}} + i\frac{i^{j+1}(j+1)! c_{j+1}}{\omega^{j+2}} + \cdots \qquad (\omega \to \infty). \tag{2.68}$$

This result follows from application of Watson's lemma (Bender and Orszag 1978) to the Laplace transform integral.

Lemma 2
The frequency responses of the lowest moment α_0 are related to $\mathsf{R}_{00}(\omega)$ by

$$\mathsf{R}_{0j}(\omega) = P_j(\omega)\mathsf{R}_{00}(\omega) - iQ_j(\omega). \tag{2.69}$$

Proof. From the recurrence relation (2.48) it is easy to show that the response defined in Eq. (2.62) satisfies the recurrence relation

$$\mathsf{R}_{0,j}(t) = \left(a_j i\frac{\partial}{\partial t} + b_j\right) \mathsf{R}_{0,j-1}(t) - c_j \mathsf{R}_{0,j-2}(t). \tag{2.70}$$

Taking the Laplace transform (2.1) and integrating by parts gives

$$\mathsf{R}_{0,j}(\omega) = (a_j\omega + b_j)\,\mathsf{R}_{0,j-1}(\omega) - c_j \mathsf{R}_{0,j-2}(\omega) - ia_n \left|\mathsf{R}_{0,j-1}(t)\right|_{t=0}. \tag{2.71}$$

Now $\mathsf{R}_{0,0}(t=0) = 1$ and $\mathsf{R}_{0,j}(t=0) = 0$ for $j \geq 1$ from the previous lemma. The recurrence equation (2.71) therefore yields

$$\begin{aligned} \mathsf{R}_{0,0}(\omega) &= 1\mathsf{R}_{0,0}(\omega) - i0, \\ \mathsf{R}_{0,1}(\omega) &= P_1(\omega)\mathsf{R}_{0,0}(\omega) - ia_1, \\ \mathsf{R}_{0,j}(\omega) &= (a_j\omega + b_j)\,\mathsf{R}_{0,j-1}(\omega) - c_j\mathsf{R}_{0,j-2}(\omega) \qquad (j > 1). \end{aligned} \tag{2.72}$$

The result follows from the fact that P_n and Q_n satisfy the recurrence relation. □

From the asymptotic behavior of $\mathsf{R}_{0m}(\omega)$ in Eq. (2.68) one can see that the formula for $\mathsf{R}_{0m}(\omega)$, Eq. (2.69), implies that

$$\mathsf{R}_{00}(\omega) - i\frac{Q_j(\omega)}{P_j(\omega)} \sim \mathcal{O}\left(\frac{1}{\omega^{2j+1}}\right) \qquad (\omega \to \infty). \tag{2.73}$$

It turns out, therefore, that the ratios $iQ_j(\omega)/P_j(\omega)$ are Padé approximations to the asymptotic series of the response function.

In fact, this relation between orthogonal polynomials and the Padé approximations for this problem is a classical result of Padé theory. There is an intimate connection between orthogonal polynomials, moments, and Padé approximations. Upon exchanging the order of integration in the definition of the frequency response (2.63), one finds that

$$\frac{i}{z}\mathsf{R}_{00}\left(-\frac{1}{z}\right) = \int_{-\infty}^{\infty} \frac{w(b)\,db}{1+zb}, \tag{2.74}$$

which is the definition of the Hamburger function for the measure $w(b)\,db$ [Eq. (6.1) of Baker and Graves-Morris (1996)]. An elementary result in the theory of the Hamburger moment problem is that the denominators of the Padé approximations to this function around $z = 0$ are just the orthogonal polynomials with respect to the measure $w(b)\,db$. The resulting Padé approximations are only guaranteed to converge for z in regions of the complex plane that are separated from the real axis by some minimum distance. Convergence for real z generally occurs only when a constant C exists such that the distribution satisfies $w(b) = 0$ for $|b| > C$, and even then is only guaranteed for $|z|$ larger than some constant.

Result 1

The general element $\mathsf{R}_{kj}(\omega)$ of the transformed response matrix is given by

$$\mathsf{R}_{kj}(\omega) = P_{\min(k,j)}(\omega)\left[P_{\max(k,j)}(\omega)\mathsf{R}_{00}(\omega) - iQ_{\max(k,j)}(\omega)\right]. \tag{2.75}$$

PROOF. Assume for the moment that $k \leq j$. The time response (2.62) may be rewritten

$$\begin{aligned} \mathsf{R}_{kj}(t) &= P_k(i\partial/\partial t)\int_{-\infty}^{\infty} e^{-ibt}P_j(b)w(b)\,db, \\ &= P_k(i\partial/\partial t)\mathsf{R}_{0j}(t). \end{aligned} \tag{2.76}$$

Recall that the Laplace transform of $(i\partial/\partial t)^n f(t)$ is just $\omega^n \widehat{f}(\omega) - i\omega^{n-1} f(0) - \cdots - f^{(n-1)}(0)$. By lemma 1 the first j derivatives of $\mathsf{R}_{0j}(t)$ vanish at $t = 0$, so the assumption $k \le j$ implies that

$$\mathsf{R}_{kj}(\omega) = P_k(\omega)\mathsf{R}_{0j}(\omega). \tag{2.77}$$

The result then follows from lemma 2. □

This expression for the exact response function is useful for deriving and evaluating the approximate response. The notation

$$\{PQ\}_{kj}(\omega) = P_{\min(k,j)}(\omega) Q_{\max(k,j)}(\omega) \tag{2.78}$$

helps to simplify the resulting expressions. The previous result becomes simply

$$\mathsf{R}_{kj}(\omega) = P_k(\omega)P_j(\omega)\mathsf{R}_{00}(\omega) - i\,\{PQ\}_{kj}(\omega). \tag{2.79}$$

2.6 Approximate Response

In matrix form, the closed linear system of orthogonal-polynomial moments becomes

$$i\mathsf{A}\begin{bmatrix} \alpha_0(\omega) \\ \alpha_1(\omega) \\ \vdots \\ \alpha_{n-1}(\omega) \end{bmatrix} = \begin{bmatrix} C_0 \\ \vdots \\ C_m \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \tag{2.80}$$

where

$$\mathsf{A} = \begin{bmatrix} -\omega - \dfrac{b_1}{a_1} & \dfrac{1}{a_1} & 0 & \dots & 0 \\ \dfrac{c_2}{a_2} & -\omega - \dfrac{b_2}{a_2} & \dfrac{1}{a_2} & \dots & 0 \\ 0 & \dfrac{c_3}{a_3} & -\omega - \dfrac{b_3}{a_3} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \dfrac{A_0}{a_n} & \dfrac{A_1}{a_n} & \dfrac{A_2}{a_n} & \dots & \dfrac{A_{n-1}}{a_n} - \omega - \dfrac{b_n}{a_n} \end{bmatrix}. \tag{2.81}$$

The fact that the initial distribution constants $\{C_0, C_1, \dots, C_m\}$ enter the problem in the equations for the first m moments only is a property of the orthogonal-polynomial-moment expansion. The solution to this matrix problem

$$\alpha_k = \sum_{j=0}^{m} \mathsf{R}^{\mathrm{a}}_{kj}(\omega) C_j \tag{2.82}$$

defines the approximate response matrix $\mathsf{R}^{\mathrm{a}} = -i\mathsf{A}^{-1}$.

Several important questions can be considered. Is there a general procedure for choosing the coefficients $\{A_0, A_1, \ldots, A_{n-1}\}$ for the n-moment system? Does the approximate response converge? Does $\mathsf{R}^{\mathrm{a}}_{kj}(\omega) \to \mathsf{R}_{kj}(\omega)$ as $n \to \infty$? Does $\mathsf{R}^{\mathrm{a}}_{kj}(t) \to \mathsf{R}_{kj}(t)$ as $n \to \infty$? The approximate response functions $\mathsf{R}^{\mathrm{a}}_{kj}(\omega)$ are Padé approximations in ω and have poles in the complex plane. Causality requires that these poles lie in the lower-half complex plane, and closures that give poles in the upper-half complex plane will generate systems that are exponentially unstable. What is the behavior of the poles of the approximate response function as a function of the number of moments? The following sections will attempt to address these questions.

2.6.1 Form and Asymptotics of the Approximate Response

Result 2

The coefficients of the approximate response matrix $\mathsf{R}^{\mathrm{a}}_{kj}(\omega)$ for the closed system of n orthogonal-polynomial moments, Eq. (2.80), are given by

$$\begin{aligned}\mathsf{R}^{\mathrm{a}}_{kj}(\omega) = &- i\left\{PQ\right\}_{kj}(\omega) \\ &+ iP_k(\omega)\frac{\{PQ\}_{nj}(\omega) - A_{n-1}\{PQ\}_{n-1,j}(\omega) - \cdots - A_0\{PQ\}_{0j}(\omega)}{P_n(\omega) - A_{n-1}P_{n-1}(\omega) - \cdots - A_0P_0(\omega)}.\end{aligned} \tag{2.83}$$

Proof. Verification that $\sum_{k=0}^{n-1} i\mathsf{A}_{mk}\mathsf{R}^{\mathrm{a}}_{kj}(\omega) = \delta_{mj}$ involves straightforward algebra. Note that

$$\frac{c_j}{a_j}\{PQ\}_{j-1,l} - \left(\omega + \frac{b_j}{a_j}\right)\{PQ\}_{j,l} + \frac{1}{a_j}\{PQ\}_{j+1,l} = \delta_{jl}, \tag{2.84}$$

follows from the recurrence relation (2.48) and the conjugacy relation (2.64). □

As with the exact response, one can attempt to relate the general approximate response to the basic response $\mathsf{R}^{\mathrm{a}}_{00}(\omega)$, which takes the form

$$\mathsf{R}^{\mathrm{a}}_{00}(\omega) = i\frac{Q_n(\omega) - A_{n-1}Q_{n-1}(\omega) - \cdots - A_0Q_0(\omega)}{P_n(\omega) - A_{n-1}P_{n-1}(\omega) - \cdots - A_0P_0(\omega)}. \tag{2.85}$$

Using the definition of $\{PQ\}_{kj}$, the general solution can be written as

$$\begin{aligned}\mathsf{R}^{\mathrm{a}}_{kj}(\omega) =& P_k(\omega)P_j(\omega)\mathsf{R}^{\mathrm{a}}_{00}(\omega) - i\{PQ\}_{kj}(\omega) \\ &+ iP_k(\omega)\frac{\sum_{r=0}^{j-1} A_r\left[P_j(\omega)Q_r(\omega) - P_r(\omega)Q_j(\omega)\right]}{P_n(\omega) - A_{n-1}P_{n-1}(\omega) - \cdots - A_0P_0(\omega)}.\end{aligned} \tag{2.86}$$

From this form of the approximate response, it is easy to obtain the first major result concerning the error in the response function defined by

$$\Delta_{kj}(\omega) = \mathsf{R}^{\mathrm{a}}_{kj}(\omega) - \mathsf{R}_{kj}(\omega). \tag{2.87}$$

Subtracting the exact response (2.79) from the approximate response (2.86) yields the following result.

Result 3
For the orthogonal-polynomial moment system with closure, setting the first p closure coefficients to zero ($A_0 = \cdots = A_{p-1} = 0$) enables the errors in the response functions corresponding to $C_0, \ldots, C_p$ to be related to each other by the formula

$$\Delta_{kj}(\omega) = P_k(\omega)P_j(\omega)\Delta_{00}(\omega) \qquad (j \leq p). \tag{2.88}$$

Fitting the basic response $\mathsf{R}_{00}(\omega)$ well therefore ensures a good fit for all the response functions $\mathsf{R}_{kj}(\omega)$ with $j \leq p$ if the first p coefficients are set to zero. Fitting those components of the response function ensures that the response to distributions of the form $\rho(b) = [C_0P_0(b) + \cdots + C_pP_p(b)]\, w(b)$ is modeled well. Increasing p therefore enables one to uniformly approximate a greater variety of initial conditions. Setting the first p coefficients to zero also ensures a good fit of the basic response in the $\omega \to \infty$ limit.

Result 4
Setting the first p closure coefficients to zero ($A_0 = \cdots = A_{p-1} = 0$) improves the asymptotic fit of the approximate response function by a factor of ω^{-p}. The approximate response behaves as

$$\mathsf{R}^{\mathsf{a}}_{00}(\omega) - \mathsf{R}_{00}(\omega) \sim \mathcal{O}\left(\frac{1}{\omega^{n+1+p}}\right) \qquad (\omega \to \infty). \tag{2.89}$$

Proof. The asymptotic result expressed in Eq. (2.73) implies that $P_j(\omega)\mathsf{R}_{00}(\omega) - iQ_j(\omega) \sim \mathcal{O}(\omega^{-(j+1)})$ as $\omega \to \infty$. The asymptotic behavior of the linear combination

$$\begin{aligned}&[P_n(\omega) - A_{n-1}P_{n-1}(\omega) - \cdots - A_pP_p(\omega)]\, \mathsf{R}_{00}(\omega)\\ &\quad - i\,[Q_n(\omega) - A_{n-1}Q_{n-1}(\omega) - \cdots - A_pQ_p(\omega)] \sim \mathcal{O}\left(\frac{1}{\omega^{p+1}}\right) \qquad (\omega \to \infty),\end{aligned} \tag{2.90}$$

is given by the worst term $A_pP_p(\omega)\mathsf{R}_{00}(\omega) - iA_pQ_p(\omega)$. The result follows using the definition of $\mathsf{R}^{\mathsf{a}}_{00}(\omega)$ in Eq. (2.85) after dividing Eq. (2.90) by the denominator of $\mathsf{R}^{\mathsf{a}}_{00}(\omega)$. $\square$

Thus there are two benefits to setting the lowest closure coefficients to zero. The asymptotic response is improved and the approximate response models initial conditions with more degrees of freedom. Why not simply take the maximum possible choice $p = n$, which corresponds to moment truncation [$\alpha_n(t) = 0$]? The resulting approximate response

$$\mathsf{R}^{\mathsf{a}}_{00}(\omega) = i\frac{Q_n(\omega)}{P_n(\omega)} \tag{2.91}$$

matches the exact response to $\mathcal{O}(\omega^{-(2n+1)})$ as $\omega \to \infty$, a significant improvement over truncation in b^n moments, which leads to the Taylor-series approximation (2.17), which matches the exact response to $\mathcal{O}(\omega^{-(n+1)})$ as $\omega \to \infty$. The denominator of this approximation, $P_n(\omega)$, is an orthogonal polynomial with respect to a positive weight function, and therefore has n zeroes on the real axis. This approximation yields solutions that are oscillatory in time and fail to model the phase-mixing decay.

2.6.2 Two-Point Approximation

The question remains how to choose the remaining coefficients if some are to be left nonzero ($p < n$). Matching in the $\omega \to \infty$ limit forces more coefficients to be zero, so some other part of the response function must be looked at. One is therefore naturally led to consider generalized Padé approximants involving other limits. Multi-point Padé approximations are sometimes called rational interpolants or Newton–Padé approximants. Various definitions exist for two-point approximants since one point may be infinite and there is a degree of freedom in how to split the total number of matching conditions between the two points. The particular definition chosen here corresponds to the problem at hand where the approximate response function is a ratio of polynomials that naturally matches the exact response in the $\omega \to \infty$ limit, and one wishes to fix coefficients by matching at a point elsewhere.

Definition 5
Suppose a function $f(z)$ has an asymptotic series and power series representation

$$f(z) = \frac{c_1}{z} + \frac{c_2}{z^2} + \cdots \qquad (z \to \infty), \tag{2.92}$$
$$f(z) = d_0 + d_1(z - z_0) + d_2(z - z_0)^2 + \cdots \qquad (z \to z_0). \tag{2.93}$$

The $[N, q]$ two-point Padé approximant to f is defined by

$$f^{[N,\,q,\,z_0]}(z) = \frac{Q^{[N,q,z_0]}(z)}{P^{[N,q,z_0]}(z)}, \tag{2.94}$$

where $Q^{[N,q,z_0]}(z)$ is a polynomial of degree $N-1$, $P^{[N,q,z_0]}(z)$ is a polynomial of degree N, $f^{[N,\,q,\,z_0]}(z) - f(z) \sim \mathcal{O}(z^{-(2N+1-q)})$ as $z \to \infty$, and $f^{[N,\,q,\,z_0]}(z) - f(z) \sim \mathcal{O}((z - z_0)^q)$ as $z \to z_0$. (There are $2N$ degrees of freedom in the choice of coefficients of the polynomials and $2N$ terms have been matched in the two series.)

With the first p closure coefficients set to zero, the approximate response

$$\mathsf{R}^{\mathrm{a}}_{00}(\omega) = i\frac{Q_n(\omega) - A_{n-1}Q_{n-1}(\omega) - \cdots - A_pQ_p(\omega)}{P_n(\omega) - A_{n-1}P_{n-1}(\omega) - \cdots - A_pP_p(\omega)}. \tag{2.95}$$

matches the exact response to order $\mathcal{O}(\omega^{n+1+p})$. The approximate response therefore becomes the $[n, q, \omega_0]$ Padé approximant to the exact response for $q = n - p$ if the q remaining coefficients can be chosen to match the first q terms of the Taylor series

$$\mathsf{R}_{00}(\omega) = r_0 + r_1(\omega - \omega_0) + r_2(\omega - \omega_0)^2 + \cdots . \tag{2.96}$$

Upon expressing the polynomials in terms of $(\omega - \omega_0)$,

$$\begin{aligned} P_j(\omega) &= P_{j,0} + P_{j,1}\omega + \cdots + P_{j,j}\omega^j \\ &= P^{\omega_0}_{j,0} + P^{\omega_0}_{j,1}(\omega - \omega_0) + \cdots + P_{j,j}(\omega - \omega_0)^j, \end{aligned} \tag{2.97}$$

one obtains the matrix equation for the remaining coefficients,

$$\left(\begin{bmatrix} r_0 & 0 & \dots & 0 \\ r_1 & r_0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ r_{q-1} & r_{q-2} & \dots & r_0 \end{bmatrix} \begin{bmatrix} P^{\omega_0}_{n-1,0} & P^{\omega_0}_{n-2,0} & \dots & P^{\omega_0}_{p,0} \\ P^{\omega_0}_{n-1,1} & P^{\omega_0}_{n-2,1} & \dots & P^{\omega_0}_{p,1} \\ \vdots & \vdots & \ddots & \vdots \\ P^{\omega_0}_{n-1,q} & P^{\omega_0}_{n-2,q} & \dots & P^{\omega_0}_{p,q} \end{bmatrix} - i \begin{bmatrix} Q^{\omega_0}_{n-1,0} & Q^{\omega_0}_{n-2,0} & \dots & Q^{\omega_0}_{p,0} \\ Q^{\omega_0}_{n-1,1} & Q^{\omega_0}_{n-2,1} & \dots & Q^{\omega_0}_{p,1} \\ \vdots & \vdots & \ddots & \vdots \\ Q^{\omega_0}_{n-1,q} & Q^{\omega_0}_{n-2,q} & \dots & Q^{\omega_0}_{p,q} \end{bmatrix} \right) \times \begin{bmatrix} A_{n-1} \\ A_{n-2} \\ \vdots \\ A_p \end{bmatrix} = \begin{bmatrix} r_0 & 0 & \dots & 0 \\ r_1 & r_0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ r_{q-1} & r_{q-2} & \dots & r_0 \end{bmatrix} \begin{bmatrix} P^{\omega_0}_{n,0} \\ P^{\omega_0}_{n,1} \\ \vdots \\ P^{\omega_0}_{n,q} \end{bmatrix} - i \begin{bmatrix} Q^{\omega_0}_{n,0} \\ Q^{\omega_0}_{n,1} \\ \vdots \\ Q^{\omega_0}_{n,q} \end{bmatrix}. \quad (2.98)$$

Definition 6
Coefficients $\{A_{n-1}, A_{n-2}, \dots, A_p\}$ *satisfying the* $\omega \to \omega_0$ *conditions of Eq. (2.98) will be called the* $[n, q, \omega_0]$ *closure. The approximate response functions obtained using these closure coefficients will be denoted by* $\mathsf{R}^{[n,\, q,\, \omega_0]}_{kj}(\omega)$ *and the response function errors by* $\Delta^{[n,\, q,\, \omega_0]}_{kj}(\omega)$.

Padé convergents often provide excellent approximations even where the asymptotic series diverges. There are no general guarantees, however, that this type of two-point Padé approximation converges or even gives reasonable results. There are several things that can go wrong with the closures generated in this fashion. First, coefficients satisfying Eq. (2.98) may fail to exist if the matrix is singular. Second, the approximate response functions may have poles in the upper-half complex plane and therefore give exponential instabilities in the time solution instead of phase-mixing decay. Third, even if reasonable response functions are produced, they may fail to match the exact response at points other than $\omega = 0$ and $\omega \to \infty$. The convergence properties of this approximation scheme will be studied numerically in the following sections for several common distributions.

2.7 Convergence of the Two-Point Approximation Closure

As will be demonstrated in the next chapter, this two-point approximation closure is a generalization of the Landau-fluid closure of Hammett and Perkins (1990). Proof of convergence of the linear theory for increasing numbers of moments does not exist for

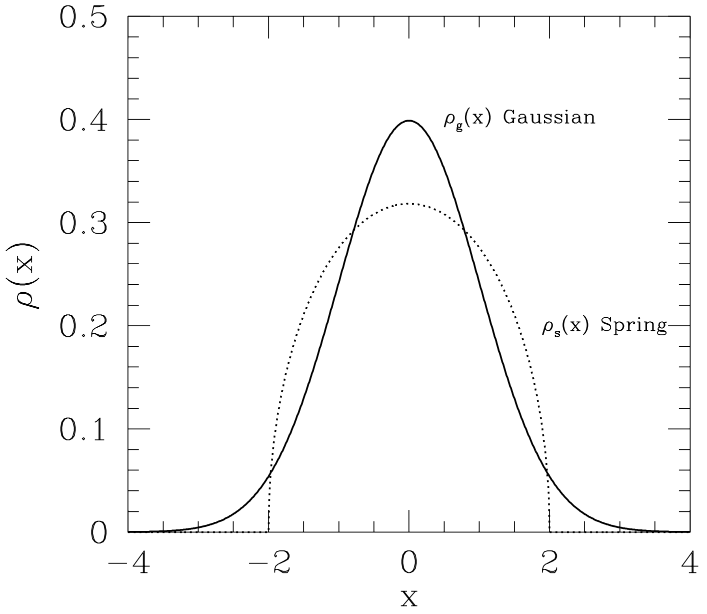

Figure 2.4: The Gaussian distribution and mass–spring distribution. Both distributions have mean 0 and variance 1.

the fluid closure problem. Here numerical evidence of convergence for these closures is presented for the two background distributions plotted in Fig. 2.4.

There is no guarantee that these closures give reasonable solutions for arbitrary n, q, and ω_0. For the subset of closures with $q = 1$, however, the two-point approximation closure yields exponentially decaying solutions that correspond to non-negative approximate distributions.

Result 5
For the general orthogonal moment linear system with positive underlying probability distribution $w(b) > 0$, the $[n, 1, \omega_0]$ closure corresponds to a non-negative approximate distribution and the resulting approximate response functions have poles that all lie in the lower half plane.

PROOF. The coefficient for the $[n, 1, \omega_0]$ closure is determined by the equation

$$\begin{aligned} 0 &= \left|\mathsf{R}_{00}(\omega) - \mathsf{R}^{\mathrm{a}}_{00}(\omega)\right|_{\omega=\omega_0} \\ &= \mathsf{R}_{00}(\omega_0) - i\frac{Q_n(\omega_0) - A_{n-1}Q_{n-1}(\omega_0)}{P_n(\omega_0) - A_{n-1}P_{n-1}(\omega_0)}. \end{aligned} \tag{2.99}$$

From the form of the response (2.63) one can show that $\mathrm{Re}(\mathsf{R}_{00}(\omega)) = \pi\, w(b)|_{b=\omega}$, so taking the real part of this equation results in

$$-A_{n-1}^i/a_n = \pi w(\omega_0)\left\{\left[P_n(\omega_0) - A_{n-1}^r P_{n-1}(\omega_0)\right]^2 + \left[A_{n-1}^i P_{n-1}(\omega_0)\right]^2\right\}. \tag{2.100}$$

[The conjugacy condition (2.64) has been used and the coefficient has been split into real and imaginary parts as $A_{n-1} = A_{n-1}^r + iA_{n-1}^i$.] The right-hand side of this equation is positive and nonzero because the zeroes of P_n and P_{n-1} are interlaced due to orthogonality. The quantity $-A_{n-1}^i/a_n$ must therefore be positive. Using the definition of the approximate distribution from Eq. (2.15) one can show that

$$\rho^{\mathrm{a}}(b) = \frac{1}{\pi}\frac{-A_{n-1}^i/a_n}{\left[P_n(b) - A_{n-1}^r P_{n-1}(b)\right]^2 + \left[A_{n-1}^i P_{n-1}(b)\right]^2}. \tag{2.101}$$

Hence, the approximate distribution for this system is defined and positive for all b. The evolution of the sum of squares of the moments

$$\frac{d}{dt}\sum_{j=0}^{n-1}|\alpha_j(t)|^2 = 2\frac{A_{n-1}^i}{a_n}|\alpha_{n-1}(t)|^2, \tag{2.102}$$

can be derived for the closed linear system (2.80) assuming $q = 1$. Any pole of the response in the upper-half complex plane would imply an exponentially growing solution, which cannot satisfy Eq. (2.102) with A_{n-1}^i/a_n negative. The squared absolute value, $\left[P_n(\omega) - A_{n-1}^r P_{n-1}(\omega)\right]^2 + \left[A_{n-1}^i P_{n-1}(\omega)\right]^2$, of the denominator of the approximate response $\mathsf{R}_{00}^{\mathrm{a}}(\omega)$ is nonzero because A_{n-1} has nonzero imaginary part and zeroes of P_n cannot coincide with zeroes of P_{n-1}. Therefore, all poles of the approximate response function must lie off the real axis in the lower-half complex plane. □

Thus for completely arbitrary background distribution, the closures with $q = 1$ are guaranteed to correspond to non-negative approximate distributions for any number of moments n. The $q = 1$ set of closures may fail to converge or converge slowly, however. There is no general theorem for closures with $q > 1$. As an example, consider the pathological bi-Gaussian density

$$w(b) = \frac{1}{\sqrt{2\pi}}\left[\frac{3}{5}\exp(-b^2/2) + 4\exp(-10^2 b^2/2)\right]. \tag{2.103}$$

The behavior of the response at $\omega = 0$ is dominated by the narrow Gaussian containing less than half the total density. The $[4, 2, 0]$ closure for this distribution was computed numerically and found to have a pole at $\sim 10.76i$ and therefore gives non-physical exponentially growing solutions and violates causality. Note that this distribution was constructed to behave strangely at the point ω_0 where the matching was done to obtain closure coefficients. For the two typical distributions considered in the following sections, all of the closures had poles confined to the lower half of the

$[n, q, \omega_0]$	closure
$[1,1,0]$	$\langle by \rangle = -i\sqrt{\frac{2}{\pi}}\langle y \rangle$
$[2,1,0]$	$\langle b^2y \rangle - \langle y \rangle = -i\sqrt{\frac{\pi}{2}}\langle by \rangle$
$[3,1,0]$	$\langle b^3y \rangle - 3\langle by \rangle = -i2\sqrt{\frac{2}{\pi}}\left(\langle b^2y \rangle - \langle y \rangle\right)$
$[3,2,0]$	$\langle b^3y \rangle - 3\langle by \rangle = -i\frac{\sqrt{2\pi}}{4-\pi}\left(\left\langle b^2y \right\rangle - \langle y \rangle\right) + \frac{3\pi-8}{4-\pi}\langle by \rangle$
$[4,1,0]$	$\langle b^4y \rangle - 6\langle b^2y \rangle + 3\langle y \rangle = -i\frac{3}{4}\sqrt{2\pi}\left(\left\langle b^3y \right\rangle - 3\langle by \rangle\right)$
$[4,2,0]$	$\langle b^4y \rangle - 6\langle b^2y \rangle + 3\langle y \rangle = -i\sqrt{2\pi}\frac{2}{3\pi-8}\left(\left\langle b^3y \right\rangle - 3\langle by \rangle\right) + \frac{32-9\pi}{3\pi-8}\left(\left\langle b^2y \right\rangle - \langle y \rangle\right)$

Table 2.3: Two-point approximation closures assuming a Gaussian weight function for some small values of n and q expressed in terms of the original b^n moments.

complex plane. This example serves as a warning, however, that it is possible to obtain unphysical results if one is not careful. Alternatively, one could expand this weight function about a Gaussian by

$$w(b) \approx \exp(-b^2/2)\sum_{j=0}^{m} C_j H_j(b/\sqrt{2}). \tag{2.104}$$

The two-point closure for the Gaussian case can then be applied to this system. By result 3 the n moment closure with a given q would correspond to allowing up to $m = n - q$ Hermite polynomials in the approximation to $w(b)$. This procedure would retain the advantages that will be observed for the Gaussian case (causality and fast convergence). In principle, any arbitrary distribution function $w(b)$ could be thus represented, though the convergence rate with n may be very slow in some cases.

The fitness of a given closure can be measured by how accurately the response function for the closed system matches the exact response. There are several choices, however, of how to measure the discrepancy. Clearly a good first requirement on the closed system is that the response function has all its poles in the lower-half complex plane. This requirement ensures that the time response decays as $t \to \infty$. As a second measure of fitness, the maximum error of the frequency response along the real axis is calculated in the following section. In applications of these closures in

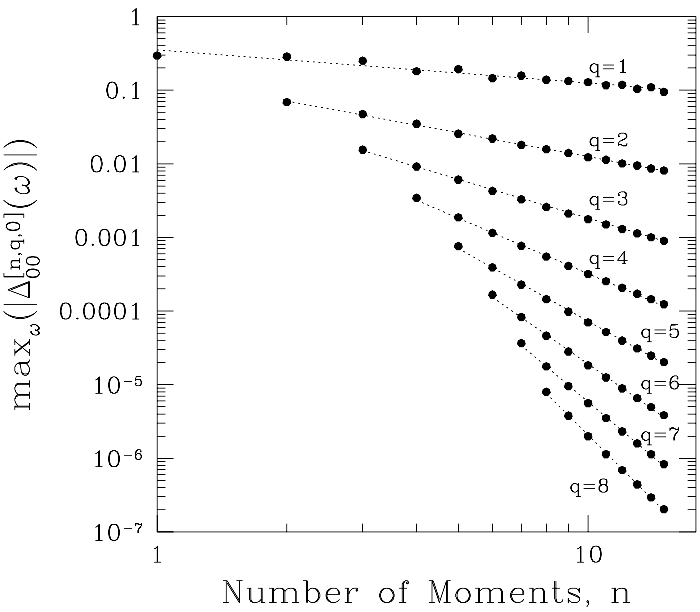

Figure 2.5: The maximum absolute error between the approximate response function and the exact response along the real axis for various two-point closures $[n, q, 0]$ in the Gaussian case is plotted against the number of moments n in the approximate system. The dotted lines are least-squares fits through the points corresponding to various choices of q, the number of times the response function is matched in the $\omega \to 0$ limit. The slopes of these fits for q from 1 through 8 are approximately $[-0.45, -1.1, -1.8, -2.5, -3.3, -4.1, -4.9, -5.8]$.

plasma physics, one is interested in accurately obtaining the growth rates of unstable modes. If the approximate response has no poles in the upper half complex plane, then the maximum modulus principle (Carrier et al. 1983, pg. 42) guarantees that the maximum error in the entire upper half plane is bounded by the maximum error along the real axis. Therefore if pointwise convergence is demonstrated on the real axis with increasing numbers of moments, the calculated growth rates for unstable modes will converge.

2.7.1 Gaussian Case

The initial study of Landau-fluid closures by Hammett and Perkins (1990) consisted essentially of application of this two-point approximation for a Gaussian distribution

$$w_G(b) = \frac{1}{\sqrt{2\pi}} \exp(-b^2/2). \tag{2.105}$$

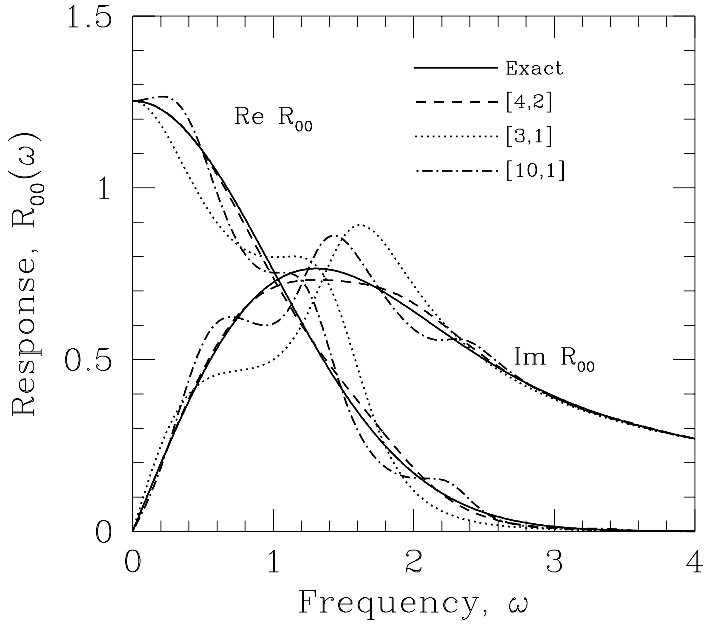

Figure 2.6: The exact response function $\mathsf{R}_{00}(\omega)$ for a Gaussian weight function (solid lines) and three of the two-point approximation closure response functions (dashed lines) corresponding to $[n=4, q=2]$, $[n=3, q=1]$ and $[n=10, q=1]$.

This case is of primary interest in plasma physics where velocities are assumed to have a Maxwellian distribution, so the frequencies $k_{\|}v$ have a Gaussian PDF. The exact response from Eq. (2.32) is just

$$\mathsf{R}_{00}(\omega) = \frac{-i}{\sqrt{2}} Z(\omega/\sqrt{2}). \tag{2.106}$$

For the Vlasov equation the initial conditions (which act as the distribution of frequencies $\rho(b)$) are of the form $bw_G(b)$. The appropriate response function to consider is

$$\mathsf{R}_{01}(\omega) = -i\left[1 + \frac{\omega}{\sqrt{2}} Z(\omega/\sqrt{2})\right]. \tag{2.107}$$

Provided closures with $p \geq 1$ are considered, however, the approximate response errors are related by $[\mathsf{R}^{\mathrm{a}}_{01}(\omega) - \mathsf{R}_{01}(\omega)] = \omega[\mathsf{R}^{\mathrm{a}}_{00}(\omega) - \mathsf{R}_{00}(\omega)]$.

Since the response function satisfies the symmetry $\mathsf{R}_{00}(-\omega) = \mathsf{R}^{*}_{00}(\omega)$, it is natural to consider $\omega_0 = 0$, in other words to match in the $\omega \to 0$ limit. For reference, some of the $[n, q, 0]$ closures are listed in Table 2.3 in terms of the original b^n moments.

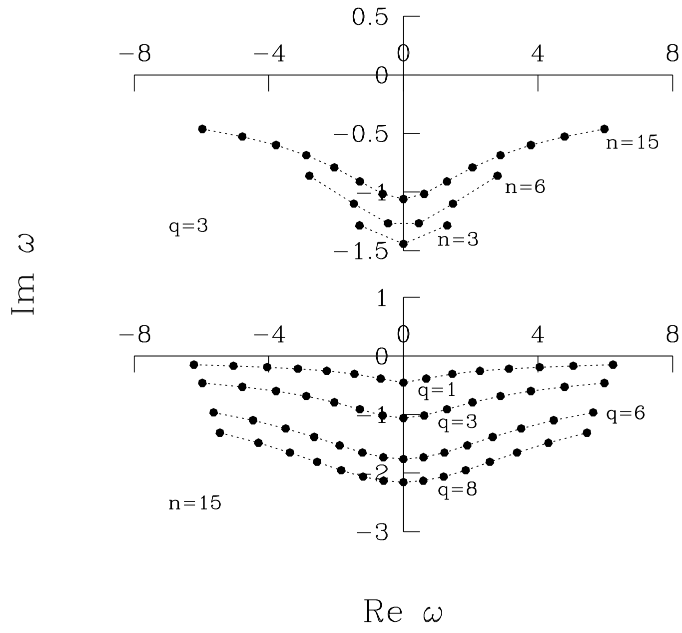

Figure 2.7: The locations in the complex plane of the poles of the approximate response function are shown for several different moment closures. In the top graph, where q is fixed at 3, the poles move towards the real axis with increasing numbers of moments. For a fixed number of moments ($n = 15$ in the lower graph), the poles move away from the real axis as q is increased.

The closures of Hammett and Perkins (1990) correspond to the $[3, 1, 0]$ and $[4, 2, 0]$ closures here.

The maximum error $\Delta_{00}(\omega)$ for real ω was computed for various closures and plotted in Fig. 2.5 against the total number of moments n. The errors seem to scale $\propto n^{-C(q)}$, where $C(q)$ is an increasing function of q. While the $q = 1$ closure have been proven to produce causal response functions, they converge poorly with increasing numbers of moments, the error scaling roughly as $n^{-0.45}$. A few of the approximate response functions are plotted in Fig. 2.6 along with the exact response. Compare the two responses from the $q = 1$ closures plotted with $n = 3$ and $n = 10$ to see the nature of the slow convergence for $q = 1$. The response from the $n = 10$ closure oscillate more around the true solution, but is only a slight improvement over that from the $n = 3$ closure. In contrast, the $[n = 4, q = 2]$ closure yields a response function that is already very close to the exact answer.

The poles of the approximate response function are plotted in the complex plane in Fig. 2.7. The upper plot shows poles for fixed $q = 3$ and three choices of n. The

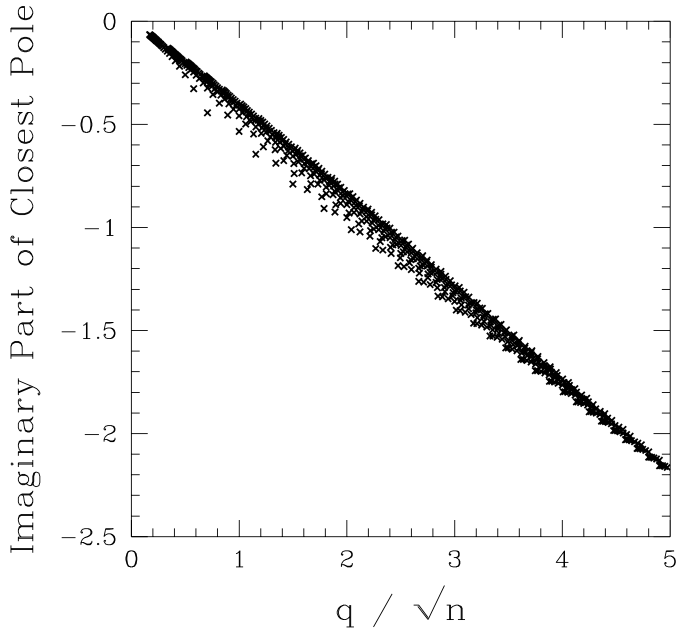

Figure 2.8: The maximum imaginary part of the poles of the $[n, q, 0]$ closure is plotted against $q/\sqrt{n}$. All closures with $1 \leq q < n \leq 35$ are included in this plot.

poles move closer to the axis with increasing number of moments and spread out. The lower plot shows poles for fixed $n = 15$ with four choices of q. The poles move away from the axis with increasing q. The response function appears to converge uniformly on the real axis as $n \to \infty$ even though the poles move progressively closer to the real axis. The distance of the closest pole to the real axis plotted in Fig. 2.8 was found empirically to scale as $q/\sqrt{n}$.

In summary, the main result obtained here is that there is strong numerical evidence that for the Gaussian case the linear response functions obtained using the two-point approximation closures converge with increasing numbers of moments. The convergence rate depends on q, the number of times the response function is matched in the $\omega \to 0$ limit. Convergence is faster for larger q. For all the cases considered, the poles lie in the lower-half complex plane, so the closures obtained in this fashion all give causal behavior.

2.7.2 Spring Response

The semi-infinite mass–spring system portrayed in Fig. (2.9) is an interesting physical model that can be used to illustrate the behavior of closures. With an infinite num-

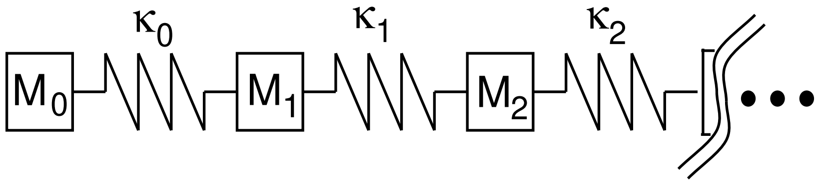

Figure 2.9: A simple one-dimensional semi-infinite mass–spring system consisting of objects, each with mass M_j, connected by springs with spring constant κ_j. The displacement of the jth mass $x_j(t)$ is measured relative to an initial state where the springs exert no forces.

ber of masses in such a system, there is a continuum of normal modes, so the system exhibits phase-mixing behavior analogous to that in the stochastic oscillator problem. The connection between the general mass–spring system and the phase-mixing problem in fluid moment equations with a Gaussian background was first illustrated by Hammett et al. (1993). Here the case with uniform spring constants $\kappa_j = \kappa$ and masses $M_j = M$ is considered as well.

The displacements of the masses $x_j(t)$ and velocities $v_j(t)$ evolve according to the equations

$$\begin{aligned} \dot{x}_0(t) &= v_0(t), \\ M_0\dot{v}_0(t) &= \kappa_0\left[x_1(t) - x_0(t)\right] \\ \dot{x}_1(t) &= v_1(t), \\ M_1\dot{v}_1(t) &= \kappa_1\left[x_2(t) - x_1(t)\right] - \kappa_0\left[x_1(t) - x_0(t)\right], \\ &\vdots \end{aligned} \tag{2.108}$$

where $\dot{f}(t)$ represents df/dt. This infinite set of equations can be written in Hamiltonian form and describes a system that is reversible and conserves energy. At low frequencies, however, this system can act like an irreversibly damped mass.

With the set of suitably normalized variables

$$\begin{aligned} \alpha_0(t) &= v_0(t), & \alpha_1(t) &= i\sqrt{\frac{\kappa_0}{M_0}}\left(x_1 - x_0\right), \\ \alpha_2(t) &= -\sqrt{\frac{M_1}{M_0}}v_1(t), & \alpha_3(t) &= -i\sqrt{\frac{\kappa_1}{M_0}}\left(x_2 - x_1\right), \\ &\vdots & &\vdots \\ \alpha_{2j}(t) &= (-1)^j\sqrt{\frac{M_j}{M_0}}v_j(t), & \alpha_{2j+1}(t) &= i(-1)^j\sqrt{\frac{\kappa_j}{M_0}}\left(x_{j+1} - x_j\right), \end{aligned} \tag{2.109}$$

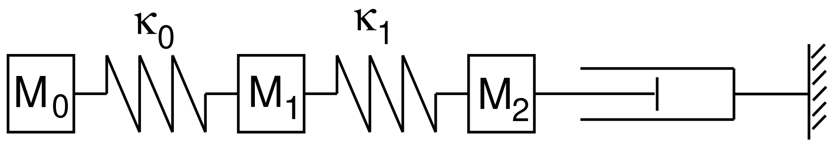

Figure 2.10: The $q = 1$ closure from the stochastic oscillator problem corresponds to adding a damping force proportional to the velocity of the last mass. This picture represents the $[5, 1]$ closure by attaching a viscous damper to the last mass.

the Laplace transform of the mass–spring system can be expressed in matrix form

$$i \begin{bmatrix} -\omega & \sqrt{\dfrac{\kappa_0}{M_0}} & 0 & 0 & 0 & \dots \\ \sqrt{\dfrac{\kappa_0}{M_0}} & -\omega & \sqrt{\dfrac{\kappa_0}{M_1}} & 0 & 0 & \dots \\ 0 & \sqrt{\dfrac{\kappa_0}{M_1}} & -\omega & \sqrt{\dfrac{\kappa_1}{M_1}} & 0 & \dots \\ 0 & 0 & \sqrt{\dfrac{\kappa_1}{M_1}} & -\omega & \sqrt{\dfrac{\kappa_1}{M_2}} & \dots \\ 0 & 0 & 0 & \sqrt{\dfrac{\kappa_1}{M_2}} & -\omega & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} \alpha_0(\omega) \\ \alpha_1(\omega) \\ \alpha_2(\omega) \\ \alpha_3(\omega) \\ \alpha_4(\omega) \\ \vdots \end{bmatrix} = \begin{bmatrix} \alpha_0(t)|_{t=0} \\ \alpha_1(t)|_{t=0} \\ \alpha_2(t)|_{t=0} \\ \alpha_3(t)|_{t=0} \\ \alpha_4(t)|_{t=0} \\ \vdots \end{bmatrix}. \tag{2.110}$$

This system is similar in form to the general linear system of orthogonal-polynomial moments, Eq. (2.80). There can be a direct correlation for a choice of spring constants and masses that correspond to the recursion coefficients of the orthogonal polynomials. For example, taking $\kappa_j = (2j+1)M_j$ and $M_j = (2j)!/4^j(j!)^2$, a series of increasingly stiffer springs and smaller masses ($M_j \sim 1/\sqrt{\pi j}$ as $j \to \infty$), gives a system of equations corresponding precisely to the Hermite moment case.

The mass–spring system provides a physical picture of the moment coupling problem. Typically one considers initial distributions that correspond to low-order moments. In the mass–spring system, such initial conditions correspond to perturbations in the left-most masses and springs. As time evolves, the distribution of $y(t)$ in the stochastic oscillator goes to finer scales in b and is therefore represented by higher-order orthogonal polynomials, which 'wiggle' more. In the mass–spring system, the initial perturbation travels as a wave to the right to masses that represent higher-order polynomials. Truncation at an odd term $[\alpha_{2n+1}(t) = 0]$ in the mass–spring system corresponds physically to cutting the nth spring and truncation at an even term $[\alpha_{2n}(t) = 0]$ corresponds to stapling the nth mass to a fixed point in space. In the truncated system, therefore, waves will reflect off the rightmost boundary and return to the low moments, unlike the semi-infinite system where waves are free to carry their energy off to infinity.

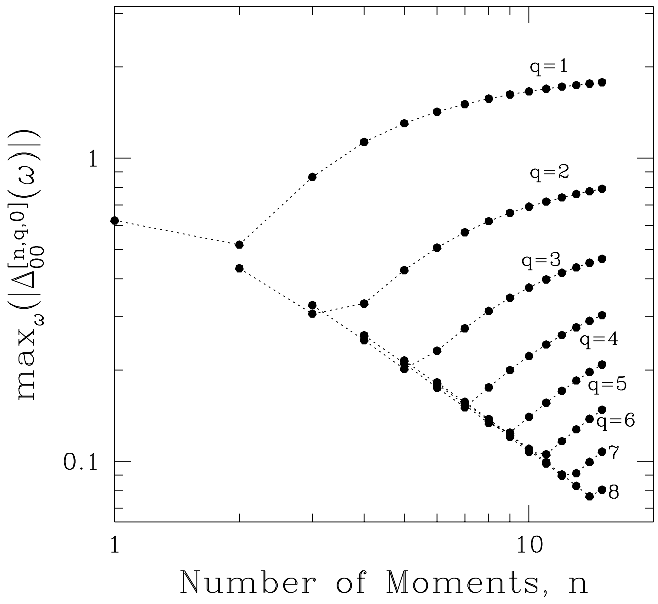

Figure 2.11: The maximum absolute error between the approximate response function and the exact response along the real axis for various two-point closures $[n, q, 0]$ for the Mass–Spring distribution is plotted against the number of moments n in the approximate system. Dotted lines connect the closures for a given q, the number of times the response function is matched in the $\omega \to 0$ limit. For fixed q the approximation improves with increasing number of moments n until $n \sim 2q$, at which point the error increases with increasing n.

The $q = 1$ closure for an odd moment $\alpha_{2n+1}(t) = -iC\alpha_{2n}(t)$ has the physical interpretation of cutting the nth spring and adding a damping force proportional to the velocity on the nth mass. The guarantee of Result 5 that solutions using the $q = 1$ closure are exponentially damped in time has a simple physical interpretation here, since the system conserves energy except for the damping term, which only removes energy from the system. Selecting the size of the damping term by matching in the $\omega \to 0$ limit is analogous to impedance matching at the end of an electrical cable. The chain of springs is a reactive system that is coupled to a dissipative element chosen to minimize the reflection of energy.

The Uniform Mass–Spring System

Consider now the case with uniform spring constants $\kappa_j = \kappa$ and masses $M_j = M$. The off-diagonal elements in the matrix system, Eq. (2.110), are then all 1. This form of the system corresponds to the recurrence relation for the polynomials $U_n(b/2)$ that

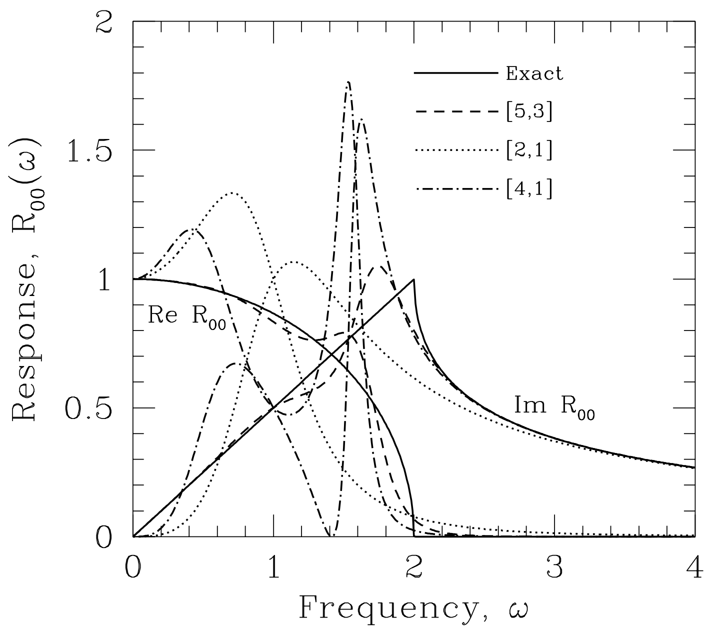

Figure 2.12: The exact response function $\mathsf{R}_{00}(\omega)$ (solid lines) for the uniform mass–spring system and three of the two-point approximation closure response functions (dashed lines) corresponding to $[n=5, q=3]$, $[n=2, q=1]$ and $[n=4, q=1]$.

are orthogonal with respect to the weight function

$$w_s(b) = \begin{cases} \dfrac{1}{\pi}\sqrt{1-(b/2)^2} & (|b|<2), \\ 0 & (|b|\geq 2), \end{cases} \tag{2.111}$$

which is plotted against a Gaussian in Fig. 2.4. This system provides an interesting test of the two-point approximation closure since the exact response to an initial velocity perturbation in the first mass,

$$\mathsf{R}_{00}(\omega) = v_0(\omega)/\left. |v_0(t)|\right|_{t=0} = \sqrt{1-(\omega/2)^2} + i\omega/2, \tag{2.112}$$

has two square-root singularities. [The square root is taken so that $\mathsf{R}_{00}(0)=1$ and by analytic continuation above the two cuts at -2 and 2 in the complex plane. At large ω, the square-root term is imaginary and cancels the linear term to leading order so that $\mathsf{R}_{00}(\omega) \sim i/\omega$.] Toroidal fluid closures must model response functions that have square-root singularities (Beer and Hammett 1996).

Again the exact response is symmetric, so the q low-frequency conditions are computed by matching in the $\omega \to 0$ limit. The maximum error along the real axis

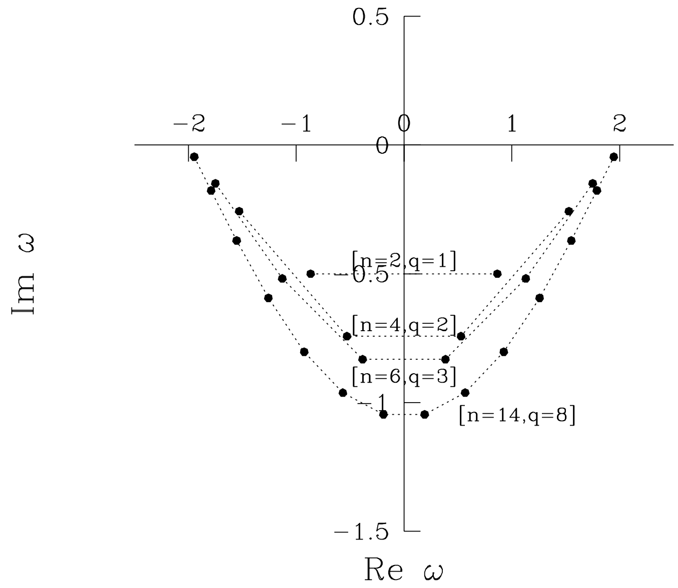

Figure 2.13: The locations in the complex plane of the poles of the approximate response functions for the mass–spring system are shown for several closures where the best q has been chosen. With increasing numbers of moments the poles move away from the real axis, with the exception of the poles at the end, which move towards the points of square-root singularity of the exact response function.

for the approximate responses is plotted in Fig. 2.11 against the number of moments n. Note the markedly different behavior in this case. With fixed q, the number of times the response is matched in the $\omega \to 0$ limit, the response functions *do not converge* with increasing numbers of moments n. For a given q, there appears to be an optimal number of moments $n \sim 2q$, beyond which the addition of extra moment equations degrades the approximation. Another way of interpreting this graph is to say that for a fixed number of moment equations n, convergence improves with increasing q until $q \sim n/2$, at which point matching additional times in the $\omega \to 0$ limits does not improve or degrade the convergence. The error does seem to scale as n^{-1}, however, for a sequence of closures such that $q > n/2$, so there can be convergence of the linear theory.

Three of the approximate responses are plotted in Fig. 2.12 along with the exact response for this system. The convergence behavior appears to be dominated by the square-root singularity at $\omega = 2$ (and $\omega = -2$). The case $[n = 4, q = 1]$ illustrates what goes wrong for $q < n/2$. The asymptotic behavior of the approximate response penetrates past the square-root singularity and gives large errors at lower ω. Matching sufficiently often in the $\omega \to 0$ limit gives more reasonable results as is demonstrated by the $[n = 5, q = 3]$ closure. The square-root singularity prevents the superb convergence obtained in the Gaussian case, however.

The poles of the response function are plotted in Fig. 2.13 for a sequence of 'optimal' closures where $n \sim 2q$. With increasing numbers of moments, there are some poles that move away from the real axis. Some of the additional poles move towards the two square-root singularities at $\omega = \pm 2$. It is reasonable to expect that convergence to response functions with such singularities will require that the approximate response function has poles near the singularities to model the non-analytic behavior there. The series of poles for a given closure can be viewed as an attempt to model the branch cuts leaving the singularities.

2.8 Summary

The issue of obtaining closures for equations evolving moments of the stochastic oscillator problem was considered here. This problem is easily solved exactly and moments exhibit *phase-mixing* decay. Simple truncation of the moment hierarchy leads to unphysical behavior as $t \to \infty$, the moments either increasing without bound (the Taylor-series approximation) or oscillating forever (for the cumulant-discard approach). The random-coupling model is a simple nonlinear closure used in fluid turbulence theories that yields decaying solutions.

A general linear closure has been introduced here, based on the Landau-fluid approach of Hammett and Perkins (1990) to obtaining fluid moment closures for collisionless plasmas. The n closure coefficients for the n-moment system are computed using conditions obtained by matching the response function for the closed moment system to the exact response function q times in the $\omega \to 0$ limit and $n - q$ times in the $\omega \to \infty$ limit. Results concerning the form of this closure are easily expressed for closures written in terms of polynomial moments where the polynomials are orthogonal with respect to the underlying distribution. A given closure for n moments is shown to match the linear response for background distributions that can be written as a polynomial of order $n - q$ in the frequency b multiplied by the given background distribution.

There is strong numerical evidence that the linear response of the closed moment system converges to the exact response for any choice of closure with increasing numbers of moments n, as long as there is some dissipation in the closure for the highest moment and the underlying distribution function is sufficiently smooth (i.e., can be represented as a Gaussian times a few low order Hermite polynomials). Convergence can be accelerated with a judicious choice of the closure dissipation, and is faster if q scales with n. However, if the underlying distribution function contains small scale features or sharp discontinuities (so its expansion in terms of Hermite polynomials requires high order polynomials), then convergence may be very slow, and a very large number of moments would be required. In some examples with sharp features in the distribution function, there was no convergence with n unless q also increased proportional to n. The poles of the approximate response functions were found to lie in the lower-half complex plane for a large number of choices of n and q.

Convergence of the response function of the closed moment system can become somewhat complicated for some underlying distributions. This approach to computing closure coefficients was applied to the semi-infinite uniform mass–spring system, which has a response function with two square-root type singularities. The response functions had well behaved poles for all the cases considered, but it appears that merely taking $n \to \infty$ does not yield converging response functions unless increasing values of q are taken as well. (The choice $q \sim n/2$ appears to work well.) The convergence properties of the semi-infinite mass–spring system indicate that care must be taken in any attempt to generalize toroidal gyrofluid equations to larger numbers of moments. The linear kinetic response function in toroidal geometry has a square-root type singularity that must be matched by the response of toroidal gyrofluid equations (Beer and Hammett 1996). In the toroidal case, the square-root branch cut is at $\omega = 0$ and so the usual method of matching the Taylor series expansion of the response at $\omega = 0$ doesn't work. Thus, Beer and Hammett (1996) chose closure coefficients to minimize the total error over a range of ω instead of only at $\omega = 0$.

2.9 Implication for Statistical Closures

The stochastic oscillator problem itself is merely a model problem. In the end, the choice of closure used for a particular problem will involve many considerations. The approach presented here is a natural one for application to fluid moment closures in plasma physics where the underlying distribution is known and numerical implementation greatly favors the lack of time history in the closure. However, when deriving closures for statistical moments in turbulence theories, one does not know ahead of time what the underlying distribution is.

In general, little is known about the convergence properties of statistical moment hierarchies in the study of turbulence. The linear results presented here are at least tangentially significant to the more general problem of nonlinear closures. The $q = 1$ closures for example, introduce a damping term in the highest moment only. The linear response for the $q = 1$ closures converges slowly for the Gaussian case and does not converge at all for the Mass–Spring problem with increasing numbers of moments even though information about the exact response is used in deriving the closure coefficient. For statistical closures in turbulence, where information about the exact nonlinear response is unavailable, one might expect even weaker convergence properties for similar closures that introduce only simple damping terms.