Path integrals and fluctuations in irreversible thermodynamics

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We express the set of stochastic differential equations which describe fluctuations in linear irreversible thermodynamics in terms of path integrals. The stochastic terms which are added to the linearized macroscopic equations have a correlation matrix that is singular, which implies that the straightforward formulation of the problem in terms of path integrals fails. We therefore begin by constructing a path-integral representation which is valid whether or not the correlation matrix is singular. We apply this to linearized irreversible thermodynamics, but the technique is designed to be applicable to more general versions of the theory. The approach emphasizes the role of the response and correlation functions as basic elements of the theory, and we calculate these quantities explicitly for the case of density fluctuations in a fluid.

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I. INTRODUCTION

The study of fluctuations in a thermodynamic context has a long history dating back to Onsager [1]. A systematic method of investigating this subject begins by forming mesoscopic equations by adding stochastic terms, representing the fluctuations, to the macroscopic thermodynamic equations. The resulting Langevin-type equations give a description of the system from which correlation functions and other quantities of interest can be calculated. The simplest such formulation, first investigated by Onsager and Machlup [2], consists of linearizing the macroscopic equations about the equilibrium state and assuming that the stochastic description is stationary, Gaussian and Markovian. This gives rise to a consistent theory of fluctuations in linear irreversible thermodynamics (LIT). The derivation of the deterministic equations of this theory is straightforward—the five balance equations for mass, linear momentum and energy are linearized—but the quantitative description of the stochastic terms requires a little more work. Since the process is Gaussian and Markovian, and since the deterministic equations are linear and first order in time, these stochastic terms should consist of Gaussian white noise with zero mean. As such they will be completely described by a noise correlation matrix $Q_{ab}, a, b=1,\ldots,5$. This matrix cannot *a priori* be determined from the macroscopic equations, but the assumption of Langevin dynamics of the type we have described, leads to a fluctuation dissipation theorem (FDT) which gives Q_{ab} in terms of a matrix which does appear in the macroscopic equations [3,4]. Thus all quantities in the theory can be determined, and quantitative predictions can now be made.

Within the past two or three decades this theory has been extended in various ways. For instance, in the formulation of extended irreversible thermodynamics (EIT) [5–8] and nonlinear irreversible thermodynamics (NLIT) [9,10]. The stochastic version of the former leads to processes which are non-Markovian if the original five variables of mass, linear momentum and energy are used [4], and the latter attempts to keep nonlinear terms in the balance equations. Performing calculations in these more complex theories is not so straightforward: if the process is not Markovian, simple forms of the Fokker-Planck equation are not available and if the Langevin equations are nonlinear, systematic approximation procedures need to be developed. In both these cases, the analysis of the theory and explicit calculations can be simplified by reformulating the Langevin equations as path integrals. This is due to the fact that the path-integral formulation of non-Markovian processes is not inherently different from that of Markovian processes [11,12] and that systematic approximation schemes in stochastic nonlinear dynamics are frequently more simple to formulate in a path-integral context [13,14]. However, there is a problem: for any theory of fluctuations in nonequilibrium thermodynamics the Q matrix will be singular, due to the fact that the continuity equation has no stochastic term associated with it. Since the structure of the Onsager-Machlup functional [15], which appears in the path-integral representation of stochastic processes, involves Q^{-1} in an essential way, the naive prescription for obtaining the path-integral formulation of nonequilibrium thermodynamics cannot be followed.

In this paper, we describe a procedure for constructing path integrals when the noise-correlation matrix is singular. We will assume that the system is described by a set of continuous variables $a_b(\boldsymbol{r},t)$ with $\boldsymbol{r}$ representing position in space, t the time, and $b=1,\ldots,N$ labeling the different variables. We will then go on to apply this formalism to LIT where $N=5$ and the $a_b(\boldsymbol{r},t)$ will have the specific interpretations of volume, velocity and temperature fluctuations. Our intention is to develop a sufficiently general formalism that it can cope with the complications of EIT and NLIT, so that it may be extended to these cases in the future. We have also tried to make the presentation reasonably self-contained, so that Sec. II reviews the standard procedure for constructing path integrals when Q is nonsingular, and Sec. III describes the modifications required when Q is singular. Technical details relevant for both these sections are given in Appendix A. The special case of LIT is discussed in Sec. IV and an explicit calculation of the response and correlation functions for the case of density fluctuations in a fluid is given. Details of this calculation are given in Appendix B. We conclude in Sec. V with a brief review of the paper and plans for future work.

II. PATH-INTEGRAL FORMALISM

Since our main motivation for the work we will describe in this section and Sec. III will be the application to the study of fluctuations in LIT, we will use a notation which we adopted previously when studying this theory [4]. In this notation the Langevin-type equations which the set of variables $a_b(\boldsymbol{r},t)$ obey are written as

$$\frac{\partial a_b(\boldsymbol{r},t)}{\partial t} = -\sum_c \int d\boldsymbol{r}' G_{bc}(\boldsymbol{r},\boldsymbol{r}') a_c(\boldsymbol{r}',t) + \tilde{f}_b(\boldsymbol{r},t). \quad (1)$$

Here the first term on the right-hand side is a result of the linearization of the macroscopic equation about the stationary state and $\tilde{f}_b(\boldsymbol{r},t)$ is a stochastic term that represents the fluctuations in the system.

So our starting point in this section will be equations of the type (1) which we will write in the form

$$\dot{a}_b^j(t) + G_{bc}^{jk} a_c^k(t) = \tilde{f}_b^j(t), \quad b,c = 1,\ldots,N, \quad (2)$$

where the continuous coordinate labels $\boldsymbol{r},\boldsymbol{r}'$ have been replaced by the discrete labels j,k for convenience and where the summation convention is assumed. The stochastic term $\tilde{f}_b^j(t)$ is taken to have a Gaussian distribution with mean zero and correlator

$$\langle \tilde{f}_b^j(t) \tilde{f}_c^k(t') \rangle = 2Q_{bc}^{jk} \delta(t-t'). \quad (3)$$

It is clear from Eq. (3) that the matrix Q, viewed in the combined (j,b) space, is real, symmetric and positive semidefinite. In this section we will review the general path-integral formalism for the case where Q is nonsingular, that is, $\det Q \neq 0$—which is in fact the general situation encountered outside the theory of fluctuating nonequilibrium thermodynamics, and was the case originally discussed by Onsager and Machlup [15].

Since the stochastic term in Eq. (2) is Gaussian, white and has zero mean, the corresponding probability distribution functional can be written as

$$\mathcal{P}[\underline{\tilde{\boldsymbol{f}}}] \sim \exp -\frac{1}{4}\int dt \tilde{f}_b^j(t) (Q^{-1})_{bc}^{jk} \tilde{f}_c^k(t), \quad (4)$$

where $\underline{\tilde{\boldsymbol{f}}} = (\underline{\tilde{f}}^1, \underline{\tilde{f}}^2, \ldots)$ and $\underline{\tilde{f}}^i = (\tilde{f}_1^i, \tilde{f}_2^i, \ldots, \tilde{f}_N^i)$. To find the probability density functional for the $\underline{\boldsymbol{a}}$ is a simple matter: the first-order differential equation (2), together with an initial condition on $a_b^j(t_0)$, defines the transformation from the functions $\tilde{f}_b^j$ to the functions a_c^k. Therefore $P[\underline{\boldsymbol{a}}] = \mathcal{P}[\underline{\tilde{\boldsymbol{f}}}]J$, where $J \equiv \mathrm{Det}(\delta\tilde{f}/\delta a)$ is the Jacobian of the transformation. Since, in this case, the relation (2) between $\underline{\tilde{\boldsymbol{f}}}$ and $\underline{\boldsymbol{a}}$ is linear, the Jacobian is independent of $\underline{\boldsymbol{a}}$ and as such can be absorbed into the normalization of $P[\underline{\boldsymbol{a}}]$. Therefore to find $P[\underline{\boldsymbol{a}}]$ we only require to substitute Eq. (2) into Eq. (4):

$$P[\underline{\boldsymbol{a}}] \sim \exp -\frac{1}{4}\int dt [\dot{a}_b^j(t) + G_{bd}^{jl} a_d^l(t)] (Q^{-1})_{bc}^{jk} \times [\dot{a}_c^k(t) + G_{ce}^{km} a_e^m(t)]. \quad (5)$$

In subsequent developments it is easier to work with Fourier transformed variables. It is shown in Appendix A that in this case Eq. (5) becomes

$$P[\underline{\boldsymbol{a}}] \sim \exp -\frac{1}{4}\int \frac{d\omega}{2\pi} a_b^j(-\omega) (B^{-1}(\omega))_{bc}^{jk} a_c^k(\omega), \quad (6)$$

where the matrix $B(\omega)$ is given by

$$B(\omega) = \mathcal{G}(\omega) Q \mathcal{G}^\dagger(\omega), \quad (7)$$

and $\mathcal{G}(\omega) = [-i\omega I + G]^{-1}$, where I is the unit matrix.

Since Q is real and symmetric, $B(\omega)$ is Hermitian: $B^\dagger(\omega) = B(\omega)$. Using $P[\underline{\boldsymbol{a}}]$ given by Eq. (6) we can now calculate quantities of interest, for example the correlation function

$$\langle a_e^l(\omega) a_f^m(-\omega) \rangle = \langle a_e^l(\omega) a_f^{*m}(\omega) \rangle = \frac{\int D\underline{\boldsymbol{a}}\, a_e^l(\omega) a_f^{*m}(\omega) \exp(-\mathcal{S})}{\int D\underline{\boldsymbol{a}} \exp(-\mathcal{S})}, \quad (8)$$

where

$$\mathcal{S} = \frac{1}{4}\int \frac{d\omega}{2\pi} a_b^{*j}(\omega) (B^{-1}(\omega))_{bc}^{jk} a_c^k(\omega). \quad (9)$$

The Jacobian and normalization factors have canceled between the numerator and the denominator. Since B is Hermitian it may be diagonalized by a unitary transformation and the Gaussian integral (8) evaluated in the standard way [14] to yield $2B_{ef}^{lm}(\omega)$. Of course, in this simple case this result may be obtained in a more straightforward manner:

$$\langle a_e^l(\omega) a_f^m(-\omega) \rangle = \mathcal{G}_{eb}^{lj}(\omega) \mathcal{G}_{fc}^{mk}(-\omega) \langle \tilde{f}_b^j(\omega) \tilde{f}_c^k(-\omega) \rangle = \mathcal{G}_{eb}^{lj}(\omega) 2Q_{bc}^{jk} \mathcal{G}_{fc}^{mk}(-\omega), \quad (10)$$

where we have used Eq. (3). Since $\mathcal{G}_{fc}^{mk}(-\omega) = \mathcal{G}_{cf}^{\dagger km}(\omega)$,

$$\langle a_e^l(\omega) a_f^{*m}(\omega) \rangle = 2B_{ef}^{lm}(\omega) \quad (11)$$

as before.

The usual result, as quoted in de Groot and Mazur [16], for example, is given as a correlation function in time. To make contact with this result, we first note that the use of the Fourier representation means that initial conditions were set in the infinitely distant past, and so averages are with respect to a stationary probability distribution: the system is "aged." It follows that the required correlation function $\langle a_e^l(t) a_f^m(t') \rangle_S$ only depends on the combination $|t-t'|$, and t' may be set to zero without loss of generality. The subscript S is present to remind us that the distribution is stationary. It is then easy to verify that this correlation function and the one appearing in Eq. (11) are Fourier transforms of each other:

$$\langle a_e^l(t)a_f^m(0)\rangle_S = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\langle a_e^l(\omega)a_f^{*m}(\omega)\rangle e^{-i\omega t}$$

$$= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\mathcal{G}_{eb}^{lj}(\omega)2Q_{bc}^{jk}\mathcal{G}_{fc}^{mk}(-\omega)e^{-i\omega t}.$$

This integral may be evaluated using the identity

$$\mathcal{G}_{ab}^{ij}(\omega) = \int_0^{\infty} d\rho\, e^{-\rho(\mathcal{G}^{-1})_{ij}^{ab}(\omega)}. \tag{12}$$

Performing the ω integration gives the familiar result [16]

$$\langle a_e^l(t)a_f^m(0)\rangle_S = 2\int_0^{\infty} d\rho\, e^{-(\rho+t)G_{ea}^{li}}Q_{ab}^{ij}e^{-\rho G_{fb}^{mj}}\ (t \geqslant 0). \tag{13}$$

The result (11) shows that (up to a factor of 2) the matrix B is the correlation function. The matrix $\mathcal{G}$, on the other hand, is the response function. To see this let us add an external deterministic force $F_b^j(t)$ to the right-hand side of Eq. (2). Then we have

$$a_b^j(\omega) = \mathcal{G}_{bc}^{jk}(\omega)(\tilde{f}_c^{\,k}(\omega) + F_c^k(\omega)).$$

Taking the average of this equation gives $\langle a_b^j(\omega)\rangle = \mathcal{G}_{bc}^{\,jk}(\omega)F_c^k(\omega)$, and so

$$\mathcal{G}_{bc}^{\,jk}(\omega) = \frac{\partial\langle a_b^j(\omega)\rangle}{\partial F_c^k(\omega)}. \tag{14}$$

It will turn out that the closest correspondence between the path integrals for the cases when Q is singular and non-singular, occurs when response fields of the kind introduced by Janssen in the functional integral formulation of critical dynamics [13] are utilized. To introduce these fields, which will be denoted as $\hat{a}_b^i$—or writing them out fully, $\hat{a}_b(\boldsymbol{r},t)$, we begin with the probability distribution functional (4) in Fourier transformed variables:

$$\mathcal{P}[\underline{\tilde{\boldsymbol{f}}}] \sim \exp - \frac{1}{4}\int\frac{d\omega}{2\pi}\tilde{f}_b^{\,j}(-\omega)(Q^{-1})_{bc}^{jk}\tilde{f}_c^k(\omega). \tag{15}$$

This can be written in the form

$$\mathcal{P}[\underline{\tilde{\boldsymbol{f}}}] \sim \int D\hat{\boldsymbol{a}}_1 D\hat{\boldsymbol{a}}_2\ldots D\hat{\boldsymbol{a}}_N \exp\int\frac{d\omega}{2\pi}[i\hat{a}_b^j(-\omega)\tilde{f}_b^j(\omega) - \hat{a}_b^j(-\omega)Q_{bc}^{jk}\hat{a}_c^k(\omega)], \tag{16}$$

since completing the square gives Eq. (15) as required. It is not surprising that this starting point is closer to that of the singular case, since now it is Q, and not Q^{-1}, which appears in the expression for $\mathcal{P}[\underline{\tilde{\boldsymbol{f}}}]$.

We can obtain a second form for $P[\underline{\boldsymbol{a}}]$ by starting from Eq. (16), and proceeding as before. Since the Jacobian is a constant, the form of $P[\underline{\boldsymbol{a}}]$ involving response fields is simply found by substituting $\tilde{f}_b^j(\omega)$ in terms of the $a_c^k(\omega)$:

$$P[\underline{\boldsymbol{a}}] \sim \int D\hat{\boldsymbol{a}}_1 D\hat{\boldsymbol{a}}_2\ldots D\hat{\boldsymbol{a}}_N \exp\int\frac{d\omega}{2\pi} \times[i\hat{a}_b^j(-\omega)(\mathcal{G}^{-1})_{bc}^{jk}(\omega)a_c^k(\omega) - \hat{a}_b^j(-\omega)Q_{bc}^{jk}\hat{a}_c^k(\omega)]. \tag{17}$$

This version of the path integral is especially useful in nonlinear theories if a perturbation expansion in the nonlinear terms has to be carried out. In this case the terms in the exponential in Eq. (17) would be the "free part" of the theory and the non-Gaussian "interacting" terms would be expanded perturbatively. Finally, we can define new response fields $\hat{a}_c'^k(\omega) = \hat{a}_b^j(\omega)(\mathcal{G}^{-1})_{bc}^{jk}(-\omega)$, so that $P[\underline{\boldsymbol{a}}]$ has the form

$$\int D\hat{\boldsymbol{a}}_1' D\hat{\boldsymbol{a}}_2'\ldots D\hat{\boldsymbol{a}}_N' \exp\int\frac{d\omega}{2\pi}[i\hat{a}_c'^k(-\omega)a_c^k(\omega) - \hat{a}_b'^j(-\omega)\{\mathcal{G}Q\mathcal{G}^{\dagger}\}_{bc}^{jk}(\omega)\hat{a}_c'^k(\omega)]. \tag{18}$$

Dropping the primes and using the definition (7) of B gives the third form for $P[\underline{\boldsymbol{a}}]$:

$$P[\underline{\boldsymbol{a}}] \sim \int D\hat{\boldsymbol{a}}_1 D\hat{\boldsymbol{a}}_2\ldots D\hat{\boldsymbol{a}}_N \exp\int\frac{d\omega}{2\pi}[i\hat{a}_c^k(-\omega)a_c^k(\omega) - \hat{a}_b^j(-\omega)B_{bc}^{jk}(\omega)\hat{a}_c^k(\omega)]. \tag{19}$$

Any of the three forms (6), (17), or (19) are valid representations for $P[\underline{\boldsymbol{a}}]$ when Q is non-singular. In Appendix A we show that the response and correlation functions are simply found as averages of the a and $\hat{a}$ fields with a weight given by the exponential factor in Eq. (17) or Eq. (19).

We shall not explore this case any further. Our aim in this section has simply been to introduce the basic background and formalism so that we can can go on to discuss the situation of real interest to us: the case where the matrix Q is singular.

III. SINGULAR CORRELATION MATRIX

As we discussed earlier, a concrete example of a situation where Q is singular appears in the theory of hydrodynamic fluctuations [3,4], where the fluctuating linearized hydrodynamical equations are of the form (1), but with one of the equations having no fluctuating force. This particular equation, which we shall take to be the first one ($b=1$), has this structure because it originated from the equation of continuity. If we set $\tilde{f}_1(\boldsymbol{r},t)=0$, or $\tilde{f}_1^j(t)=0$ in the notation of Eq. (2), then it follows from Eq. (3) that $Q_{ab}^{ij}=0$ if a or b take on the value 1, that is, $Q_{ab}^{ij}(a,b=1,\ldots,N)$ has the form

$$Q = \begin{pmatrix} 0 & \ldots & 0 \\ & Q_{\alpha\beta}^{ij} & \\ 0 & & \end{pmatrix} \tag{20}$$

with $\alpha,\beta=2,\ldots,N$ (Greek letters will run from 2 to N and Roman letters from 1 to N). We will begin the study of this singular case by exploiting the linear nature of the problem to obtain the relation analogous to Eq. (11) and then move on to the discussion of the construction of several forms of the path integral when Q is singular.

We begin by noting that the Fourier transform of the first of the equations (2) with $\tilde{f}^{\,i}_{\;1}=0$ is

$$[-i\omega\delta^{jk}+G^{jk}_{11}]a^k_1(\omega)+G^{jk}_{1\gamma}a^k_\gamma(\omega)=0 \tag{21}$$

$$\Rightarrow a^i_1(\omega)=-g^{ij}(\omega)G^{jk}_{1\gamma}a^k_\gamma(\omega), \tag{22}$$

where g^{ij} is the inverse of the matrix $[-i\omega\delta^{ij}+G^{ij}_{11}]$ [this should not be confused with the matrix $\mathcal{G}^{ij}_{11}$, which is the $(a,b)=(1,1)$ component of the inverse of $(\mathcal{G}^{-1})^{ij}_{ab}$]. The other $(N-1)$ equations read

$$[-i\omega\delta^{jk}\delta_{\beta\gamma}+G^{jk}_{\beta\gamma}]a^k_\gamma(\omega)+G^{jk}_{\beta 1}a^k_1(\omega)=\tilde{f}^j_\beta \tag{23}$$

which implies that

$$[-i\omega\delta^{jk}\delta_{\beta\gamma}+G^{jk}_{\beta\gamma}-G^{jl}_{\beta 1}g^{li}(\omega)G^{ik}_{1\gamma}]a^k_\gamma(\omega)=\tilde{f}^j_\beta(\omega). \tag{24}$$

From Eqs. (22) and (24), it is clear that $a^j_1(t)$ will be a stochastic variable, since the $a^j_\beta(t)$ are. While the relations (22) and (24) between the a^j_b and the $\tilde{f}^j_\beta$ look to be quite complicated, the inverse relations are very simple. This can be seen by starting from the result $a^j_b(\omega)=\mathcal{G}^{jk}_{bc}(\omega)\tilde{f}^{\,k}_{\;c}$ discussed earlier (valid for nonsingular systems) and setting $\tilde{f}^{\,k}_{\;1}=0$. This yields

$$a^j_b(\omega)=\mathcal{G}^{jk}_{b\gamma}(\omega)\tilde{f}^{\,k}_{\;\gamma}. \tag{25}$$

For clarity let us apply this to a simple situation, namely the case $N=2$. Of course, this does not directly correspond to a thermodynamic problem, but it is sufficiently simple that everything may be written down explicitly in a straightforward way. Dropping the j and k (spatial) indices for clarity, Eqs. (2) and (20) become

$$\dot{a}_1(t)+G_{11}a_1(t)+G_{12}a_2(t)=0,$$

$$\dot{a}_2(t)+G_{21}a_1(t)+G_{22}a_2(t)=\tilde{f}_2(t), \tag{26}$$

and

$$Q=\begin{pmatrix}0 & 0\\ 0 & Q_{22}\end{pmatrix}. \tag{27}$$

Taking Fourier transforms, the first equation in Eq. (26) is a special case of Eq. (21):

$$[-i\omega+G_{11}]a_1(\omega)+G_{12}a_2(\omega)=0, \tag{28}$$

from which we may obtain an expression for $a_1(\omega)$, as in Eq. (22):

$$a_1(\omega)=-g(\omega)G_{12}a_2(\omega). \tag{29}$$

Here $g(\omega)$ is the inverse of $[-i\omega+G_{11}]$. Substituting Eq. (29) into the second equation in Eq. (26) yields

$$[-i\omega+G_{22}-G_{21}g(\omega)G_{12}]a_2(\omega)=\tilde{f}_2(\omega), \tag{30}$$

which should be compared with Eq. (24). Even in this the simplest case, it is clear that eliminating the a_1 variable leads to a complicated expression for a_2 [and also, from Eq. (29), for a_1]. Therefore it is better not to break the symmetry of the problem by picking out the a_1 variable as special, and instead use the inverse relations which express the a's in terms of f_2:

$$a_1(\omega)=\mathcal{G}_{12}(\omega)\tilde{f}_2,\quad a_2(\omega)=\mathcal{G}_{22}(\omega)\tilde{f}_2. \tag{31}$$

It is straightforward to invert the matrix $[-i\omega+G]$, in this simple case, to find $\mathcal{G}$ and so show, for instance, that

$$[-i\omega+G_{22}-g(\omega)G_{21}G_{12}]\mathcal{G}_{22}=1.$$

Returning to the general case, it is now simple to use Eq. (25) to obtain the analogous results to Eqs. (10) and (11):

$$\begin{aligned}\langle a^l_e(\omega)a^m_f(-\omega)\rangle &= \mathcal{G}^{lj}_{e\beta}(\omega)\mathcal{G}^{mk}_{f\gamma}(-\omega)\langle\tilde{f}^j_\beta(\omega)\tilde{f}^{\,k}_{\;\gamma}(-\omega)\rangle\\ &= 2\mathcal{G}^{lj}_{e\beta}(\omega)Q^{jk}_{\beta\gamma}\mathcal{G}^{\dagger km}_{\gamma f}(\omega),\end{aligned} \tag{32}$$

where we have used Eq. (3). We now observe that from Eq. (7), $B^{lm}_{ef}=\mathcal{G}^{lj}_{eb}Q^{jk}_{bc}\mathcal{G}^{\dagger km}_{cf}$, which becomes in the singular case (20), when all elements of Q having a subscript one vanish,

$$B^{lm}_{ef}=\mathcal{G}^{lj}_{e\beta}Q^{jk}_{\beta\gamma}\mathcal{G}^{\dagger km}_{\gamma f}, \tag{33}$$

and therefore Eq. (32) becomes

$$\langle a^l_e(\omega)a^{*m}_f(\omega)\rangle=2B^{lm}_{ef}(\omega) \tag{34}$$

exactly the same as the nonsingular analog (11).

After this preliminary discussion we can now go on to discuss how the path integrals are modified when Q is singular. Whereas our previous discussion relied on solving linear equations for $a^j_b(\omega)$, we will construct the path integrals in a way which generalizes easily to the case where the original equations (2) are nonlinear. We will then specialize to the linear case to show that results such as Eq. (34) are recovered. In the singular case, the functional (4) is replaced by

$$\mathcal{P}[\underline{\tilde{f}}]\sim\left(\prod_{t,i}\delta(\tilde{f}^{\,i}_{\;1}(t))\right)\exp-\frac{1}{4}\int dt\tilde{f}^j_\beta(t)(Q^{-1})^{jk}_{\beta\gamma}\tilde{f}^{\,k}_{\;\gamma}(t). \tag{35}$$

The probability density functional $P[\underline{a}]$ for this case can be written in a number of ways. In the singular case it is useful to still view the transformation from the functions $\tilde{f}^j_b$ to the functions a^k_c to be as before, that is, given by Eq. (2), but with the added constraint that $\tilde{f}^j_1=0$. So the Jacobian is again constant due to the linear nature of the transformation, and in the transformed variables the constraint becomes $(\mathcal{G}^{-1})^{jk}_{1b}a^k_b=0$. Since Eq. (35) only involves $\tilde{f}^j_2,\ldots,\tilde{f}^j_N$ in the exponential, we may use Eq. (24) to eliminate them in exactly the same way as in Sec. II. The construction now proceeds by analogy with Eq. (5) in the nonsingular case but with b and c replaced by β and γ respectively, and using the fact that the inverse (in the subspace defined by the Greek indices) of the matrix multiplying a^k_γ in Eq. (23) is $\mathcal{G}^{jk}_{\beta\gamma}$. One finds

$$\begin{aligned}P[\underline{a}]\sim&\left(\prod_{\omega,i}\delta((\mathcal{G}^{-1})^{ij}_{1b}(\omega)a^j_b(\omega))\right)\exp-\frac{1}{4}\int\frac{d\omega}{2\pi}a^{*j}_\beta(\omega)\\ &\times(B^{-1}(\omega))^{jk}_{\beta\gamma}a^k_\gamma(\omega).\end{aligned} \tag{36}$$

A Lagrange multiplier may now be introduced to implement the constraint in Eq. (36):

$$P[\underline{\boldsymbol{a}}] \sim \int D\hat{\boldsymbol{a}}_1 \exp - \frac{1}{4} \int \frac{d\omega}{2\pi} [a^{*j}_{\beta}(\omega)(B^{-1}(\omega))^{jk}_{\beta\gamma} a^k_{\gamma}(\omega) - 4i\hat{a}^i_1(-\omega)(\mathcal{G}^{-1})^{ij}_{1b}(\omega)a^j_b(\omega)]. \quad (37)$$

This is the first form for $P[\underline{\boldsymbol{a}}]$. The analysis we have carried out easily generalizes in the case where the starting equations (2) are nonlinear—we have not used the linearity of the equations in any essential way in the procedure outlined above. If the equations are in fact nonlinear, then the first term in the exponential in Eq. (37) will contain powers of a higher than two and the second term will be of the form of $\hat{a}_1$ multiplied by a factor containing powers of a higher than one. The Jacobian factor will also cease to be a constant and become a function of the a's and will give rise to a third term in the exponential [14].

The quantity $\hat{a}^i_1$ is nothing else but a response field of the kind introduced in Sec. II. We can see this most easily by writing the probability density functional in Eq. (35) as

$$\mathcal{P}[\underline{\tilde{\boldsymbol{f}}}] \sim \left(\prod_{\omega,i} \delta(\tilde{f}^{\,i}_1(\omega))\right) \int D\hat{\boldsymbol{a}}_2 \ldots D\hat{\boldsymbol{a}}_N \exp \int \frac{d\omega}{2\pi} \times [i\hat{a}^j_{\beta}(-\omega)\tilde{f}^j_{\beta}(\omega) - \hat{a}^j_{\beta}(-\omega)Q^{jk}_{\beta\gamma}\hat{a}^k_{\gamma}(\omega)] \sim \int D\hat{\boldsymbol{a}}_1 D\hat{\boldsymbol{a}}_2 \ldots D\hat{\boldsymbol{a}}_N \exp \int \frac{d\omega}{2\pi} [i\hat{a}^j_b(-\omega)\tilde{f}^j_b(\omega) - \hat{a}^j_{\beta}(-\omega)Q^{jk}_{\beta\gamma}\hat{a}^k_{\gamma}(\omega)]. \quad (38)$$

By completing the square in the exponential in the first term on the right-hand side of Eq. (38), we see that we recover Eq. (35). The second term follows by implementing the constraint as a Lagrange multiplier in exactly the same way as was done to obtain Eq. (37) above.

This form for $\mathcal{P}[\underline{\tilde{\boldsymbol{f}}}]$ should be compared with the equivalent result (16) which holds when Q is nonsingular. In that case there was no constraint and so it is immediately apparent that the relation between the path integrals in the singular and nonsingular cases is especially clear if either of the starting forms (16) or (38) are used rather than Eqs. (4) or (35): it is necessary only to substitute Eq. (20) into Eq. (16) to obtain Eq. (38).

For clarity is it useful to again go to the case $N=2$ to see explicitly what this means in this simple case. The term in the exponent in Eq. (16)—whether the matrix Q is singular or not—is

$$i\hat{a}_1(-\omega)\tilde{f}_1(\omega) + i\hat{a}_2(-\omega)\tilde{f}_2(\omega) - \hat{a}_b(-\omega)Q_{bc}\hat{a}_c(\omega), \quad (39)$$

where $b,c=1$, 2. If the matrix has the form (27), then the last term in Eq. (39) equals $-\hat{a}_2(-\omega)Q_{22}\hat{a}_2(\omega)$ and the $\hat{a}_1$ integration may be performed to give back the constraint $\tilde{f}_1=0$. Therefore Eq. (39) applies to both the singular and nonsingular cases, as may be used as the starting point for further analysis in both situations.

The second and third forms (17) and (19) for $P[\underline{\boldsymbol{a}}]$ can be obtained in a similar way to the nonsingular case, since Eq. (38) is just a special case of Eq. (16) which applies when Q has zero entries in the first row and column. Any of the three forms (37), (17), or (19) are valid representations for $P[\underline{\boldsymbol{a}}]$ when Q is singular, but in the last two cases it is understood that one has to substitute the form (20) in order to obtain the singular version of the result. Once again, it is straightforward to obtain the result (11) from, for instance, the last of these forms, and more generally response and correlation functions can be naturally expressed as averages over the a and $\hat{a}$ fields, as discussed in Appendix A.

It is clear that these considerations can be extended in a straightforward way to the case where M of the N equations (2) have no fluctuating force: $\tilde{f}^j_1(t)=\cdots=\tilde{f}^j_M(t)=0$. Although we are not aware of previous discussions along the lines given above, the path-integral formulation of stochastic differential equations when the noise-correlation matrix is singular has been discussed in a different context—when the noise in not white (in time). For certain types of noise (for example, exponentially correlated noise, quasimonochromatic noise,…), the non-Markovian process may be written as a Markovian process in a higher dimensional space, but with a singular noise-correlation matrix [17]. However, the approach adopted in these cases—to eliminate the equations with no fluctuating forces in favor of a set of equations which all have fluctuating forces, but which may be higher order in time [18]—is not an option open to us if the equations are nonlinear. Since we wish to keep our treatment as general as possible, it is preferable to proceed as we have done here and to use a constraint to implement the condition $\tilde{f}^j_1(t)=0$. In addition, Gaussian integrals with noninvertible quadratic forms are encountered when studying fluctuations around instanton solutions. These are due to zero modes which are created due to the breaking of continuous symmetries (spatial, temporal or internal) by choosing a particular "position" for the instanton. The solution in this case is to treat the zero modes exactly through the use of collective coordinates [19], but treat the other modes in the Gaussian approximation in the usual way.

We now go on to discuss the specific case of fluctuations in LIT.

IV. FLUCTUATIONS IN LINEAR IRREVERSIBLE THERMODYNAMICS

Using hydrodynamic language, the five independent variables in LIT are the volume per unit mass v, the three components of the barycentric velocity v_{μ}, and the temperature T [16]. Linearizing about the equilibrium state $(v,v_{\mu},T)=(v_0,0,T_0)$ gives volume and temperature fluctuations defined by $v_1=v-v_0$ and $T_1=T-T_0$. We will use the same notation for the velocity and the velocity fluctuations, since no confusion should arise. It is convenient to define the actual variables we will use to be scaled versions of v_1,v_{μ} and T_1. The scaling we choose simplifies the results and is such that all the variables have the same dimension. Specifically, we define [3,4]

$$a_1 = -\rho_0^{3/2}v_1, \quad a_{\mu+1} = \left(\frac{\rho_0}{A}\right)^{1/2} v_{\mu}, \quad a_5 = \left(\frac{\rho_0 C}{T_0 A}\right)^{1/2} T_1, \quad (40)$$

where ρ_0 is the mass density in equilibrium and A and C are quantities defined solely in terms of the fluid in equilibrium:

$$A \equiv \left(\frac{\partial p}{\partial \rho}\right)_T, \quad C \equiv \left(\frac{\partial u}{\partial T}\right)_v. \tag{41}$$

Here p is the thermodynamic pressure and u is the internal energy per unit mass.

Having defined these variables, it is now straightforward to linearize the balance equations for mass, linear momentum, and energy to obtain, in the notation that we have used in this paper,

$$\dot{a}_b^j(t) + G_{bc}^{jk} a_c^k(t) = 0, \quad b,c = 1,\ldots,5. \tag{42}$$

Before giving the explicit form of the matrix G, we first remark that it is sometimes convenient to decompose it into its symmetric and antisymmetric parts:

$$G_{bc}^{jk} = S_{bc}^{jk} + A_{bc}^{jk}, \tag{43}$$

where

$$S_{bc}^{jk} = S_{cb}^{kj} \text{ and } A_{bc}^{jk} = -A_{cb}^{kj}. \tag{44}$$

The reason for this is that the FDT shows that Q is directly proportional to S [3,4]:

$$Q_{bc}^{jk} = \frac{k_B T_0}{A} S_{bc}^{jk}. \tag{45}$$

Therefore giving explicit expressions for the matrices S and A means that fluctuating LIT is completely defined.

In fact, it is the matrices $\mathcal{G}$ and B, rather than S and A which naturally occur in a path-integral context. This is because, as discussed in Appendix A, $\mathcal{G}$ and B are averages over products of the fields a and $\hat{a}$. It is clear that knowing $\mathcal{G}$ and B also completely specifies LIT, since if they are given, G and Q, and hence S and A, can be found. Therefore, when using the path-integral formulation, it is frequently more useful to write the FDT (45) in a different form which involves the matrices B and $\mathcal{G}$. To derive this alternative form we start from the definition of B given by Eq. (7) and substitute for Q using the FDT (45) to obtain

$$B(\omega) = \mathcal{G}(\omega)\left(\frac{k_B T_0}{2A}\right)[G + G^T]\mathcal{G}^T(-\omega).$$

But $\mathcal{G}(\omega)G = I + i\omega\mathcal{G}(\omega)$, and so

$$B(\omega) = \left(\frac{k_B T_0}{2A}\right)[\mathcal{G}(\omega) + \mathcal{G}^\dagger(\omega)]. \tag{46}$$

This equation tells us that the correlation function is not independent of the response function; if we can find the latter then we can determine the former. So the analysis of fluctuations in LIT reduces to inverting $[-i\omega I + G]^{-1}$ to obtain $\mathcal{G}$.

To carry out this inversion, we first need to specify the matrix G. To do this we first need to go back to the continuous coordinate labels $\boldsymbol{r},\boldsymbol{r}'$ rather than the discrete labels j,k. It is also convenient to go over to a Fourier representation in space, as well as in time. From the paper by Fox and Uhlenbeck we find that [3]

$$G(\boldsymbol{k}) = \begin{pmatrix} 0 & ic_1 k_\mu & 0 \\ ic_1 k_\mu & c_3 k_\mu k_\nu - c_4 k^2 \delta_{\mu\nu} & ic_2 k_\mu \\ 0 & ic_2 k_\mu & c_5 k^2 \end{pmatrix}, \tag{47}$$

where the constants $c_1,\ldots,c_5$ are given by

$$c_1 = A^{1/2}, \quad c_2 = \left(\frac{B}{\rho_0}\right)\left(\frac{T_0}{C}\right)^{1/2},$$

$$c_3 = \frac{(2\mu + \zeta)}{\rho_0}, \quad c_4 = \frac{2\mu}{3\rho_0},$$

$$c_5 = \frac{\lambda}{\rho_0 C}. \tag{48}$$

The constants A and C have been defined previously in Eq. (41), as have the mass density and temperature in equilibrium, ρ_0 and T_0. In addition, $B = (\partial p/\partial T)_v$ and λ, ζ and μ are the thermal conductivity, the bulk viscosity, and the shear viscosity, respectively. In fact by definition $A = c_T^2$, where c_T is the isothermal speed of sound and $C = C_v$, the specific heat at constant volume. We also have $B = \alpha/\kappa_T$, where $\alpha = (1/v)(\partial v/\partial T)_p$ and $\kappa_T = -(1/v)(\partial v/\partial p)_T$ are the thermal expansion coefficient and the isothermal susceptibility, respectively.

The inversion of $[-i\omega + G]^{-1}$ is carried out in Appendix B. For definiteness, we will consider the case of density fluctuations in a fluid, and so will wish to calculate the density-density correlation function $\langle \rho_1(\boldsymbol{k},\omega)\rho_1(-\boldsymbol{k},-\omega)\rangle$. From Eq. (40), $a_1 = -\rho_0^{3/2} v_1$, where $v_1 = -\rho_1/\rho_0^2$. Therefore

$$\begin{aligned}\langle \rho_1(\boldsymbol{k},\omega)\rho_1(-\boldsymbol{k},-\omega)\rangle &= \rho_0 \langle a_1(\boldsymbol{k},\omega) a_1(-\boldsymbol{k},-\omega)\rangle \\ &= 2\rho_0 B_{11}(\boldsymbol{k},\omega),\end{aligned} \tag{49}$$

using Eq. (11). Use of the FDT (46) then gives

$$\langle \rho_1(\boldsymbol{k},\omega)\rho_1(-\boldsymbol{k},-\omega)\rangle = \frac{k_B \rho_0 T_0}{A}[\mathcal{G}_{11}(\boldsymbol{k},\omega) + \mathcal{G}_{11}^*(\boldsymbol{k},\omega)]. \tag{50}$$

From Appendix B we have

$$\mathcal{G}_{11}(\boldsymbol{k},\omega) = \frac{(-i\omega)^2 + H_1(-i\omega) + H_2}{(-i\omega)^3 + H_1(-i\omega)^2 + H_3(-i\omega) + H_4}, \tag{51}$$

where

$$H_1 = [(c_3 - c_4) + c_5]k^2,$$

$$H_2 = [(c_3 - c_4)c_5 k^2 + c_2^2]k^2,$$

$$H_3 = H_2 + c_1^2 k^2,$$

$$H_4 = c_5 c_1^2 (k^2)^2. \tag{52}$$

From Eq. (52) we see that the constants $c_1,\ldots,c_5$ only appear in the combinations

$$c_1^2 = c_T^2, \quad c_2^2 = \frac{\alpha^2 T_0}{\kappa_T^2 \rho_0^2 C_v} = (\gamma - 1)c_T^2,$$

$$c_3 - c_4 = \frac{(4/3)\mu + \zeta}{\rho_0}, \quad c_5 = \frac{\lambda}{\rho_0 C_v}, \tag{53}$$

where $\gamma = C_p/C_v$. To derive the result $c_2^2 = (\gamma - 1)c_1^2$ we have used the equilibrium thermodynamic relations $C_p - C_v = TV\alpha^2/\kappa_T$ and $c_T^2 = 1/\rho\kappa_T$. From Eqs. (50) and (51) we obtain

$$\langle \rho_1(\boldsymbol{k},\omega)\rho_1(-\boldsymbol{k},-\omega)\rangle = \frac{2k_B\rho_0 T_0[(c_3 - c_4)\omega^2 + c_5 H_2](k^2)^2}{\omega^2(\omega^2 - H_3)^2 + (H_1\omega^2 - H_4)^2}, \tag{54}$$

where we have used $c_1^2 = A$. This agrees with the expression given in the literature [20], obtained by a very different method. If it is assumed that both $(c_3 - c_4)$ and c_5 are very small compared with $(c_1^2 + c_2^2)$, then the poles of the response function (51) are found to be at $\omega \approx -i(\gamma^{-1}c_5)k^2$ and at $\omega \approx \pm(c_1^2 + c_2^2)k^2 - (i/2)[c_3 - c_4 + c_5 - \gamma^{-1}c_5]k^2$ [20]. These give rise to Lorentzian line shapes in Eq. (54) which are the Rayleigh peak and the Brillouin doublet respectively.

In the case of many fluids $\alpha \approx 0$ which implies $C_p \approx C_v$ (or $\gamma \approx 1$) and so we may work within an approximation in which we take $c_2 = 0$. This allows us to factor a term $[-i\omega + c_5 k^2]$ from both the numerator and denominator of Eq. (51) to obtain

$$\mathcal{G}_{11}(\boldsymbol{k},\omega) = \frac{(-i\omega) + (c_3 - c_4)k^2}{(-i\omega)^2 + (c_3 - c_4)k^2(-i\omega) + c_1^2 k^2}. \tag{55}$$

The constant c_5 no longer appears in the expression for the response function and therefore the thermal conductivity does not enter into the final expression for the density-density correlation function, which is found from Eq. (50) to be

$$\begin{aligned}\langle \rho_1(\boldsymbol{k},\omega)\rho_1(-\boldsymbol{k},-\omega)\rangle &= \frac{2k_B\rho_0 T_0(c_3 - c_4)(k^2)^2}{(\omega^2 - c_1^2 k^2)^2 + \omega^2(c_3 - c_4)^2(k^2)^2} \\ &= \frac{2k_B T_0[(4/3)\mu + \zeta](k^2)^2}{(\omega^2 - c_T^2 k^2)^2 + (\omega^2/\rho_0^2)[(4/3)\mu + \zeta]^2(k^2)^2},\end{aligned} \tag{56}$$

using the physical values (53). This agrees with the result of a previous calculation [21], which again used a different method of determining this correlation function. Now the poles of Eq. (55) are at $\omega \approx \pm c_1^2 k^2 - (i/2)[c_3 - c_4]k^2$, and give rise to the Brillouin doublet only.

Our purpose in this section has been to give explicit forms for the response and correlation functions in order to illustrate what is required to carry out a calculation in practice. As we have shown, all that is needed is the inversion of a matrix. This is a simple algorithmic task, which can easily be programmed if necessary.

V. CONCLUSIONS

This paper has been concerned with the reformulation of theories of fluctuating irreversible thermodynamics in terms of path integrals. Although this was, in principle, the topic of the famous papers by Onsager and Machlup [2,15], their path-integral formalism did not cover the case where the noise correlation matrix is singular, which is exactly the case encountered in fluctuating irreversible thermodynamics.

As with any linear theory, the use of path integrals is not strictly necessary, since all calculations may be carried out directly. This is certainly the case with fluctuations in LIT, which was the specific illustrative example which we used here. However, our aim was to set up the formalism in as general a way as possible, so that it may be applied to more nontrivial theories of fluctuating irreversible thermodynamics in the future. As an example, we used a Lagrange multiplier to impose the constraint resulting from the deterministic equation without a stochastic term. This resulted in a field which was in fact an example of the response fields introduced into the functional integral formulation of critical dynamics [13]. We could have avoided this by exploiting the linear nature of the theory, and simply solved this constraint and incorporated it into the other stochastic equations. We avoided doing this, simply because it would not generalize to the case of theories with nonlinearities.

In fact the formalism of response fields proves to be a very natural one when dealing with theories with a singular noise correlation matrix. The main reason is because it is Q, not Q^{-1} which appears in this formalism, and so it is immediately applicable whether Q is singular or not. It is also useful because the average $\langle a\hat{a}\rangle$ is just the response function. In LIT there is a FDT which states that the density-density correlation function is just the real part of the corresponding response function (up to a constant), and so it is only necessary to calculate this response function. It is obtained by inverting a 5×5 matrix, which is relatively straightforward to accomplish since the inverse only has 7 independent entries due to the symmetry of the problem. The resulting expression for the correlation function, given in the case of a fluid by Eq. (54), is completely general. This approach to the calculation of the correlation function, which involves a single matrix inversion, is not the usual technique that is adopted, but it is very natural in the path-integral context, and is also very systematic. If necessary, algebraic manipulation programs could be used to invert larger and more complicated matrices.

It is hoped that the ideas contained in this paper will form the basis for investigations of more complex theories, such as EIT and NLIT, where we expect that the systematic nature of the approach will lead to a more efficient calculational method. We hope to discuss the extension of the current work to these cases in a future publication.

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APPENDIX A: SOME ASPECTS OF THE PATH-INTEGRAL FORMALISM

In this appendix we present some technical details related to the path-integral formalism of Sec. II and Sec. III.

We begin by obtaining Eq. (6) from Eq. (4) by working with the Fourier transformed variables:

$$a_c^k(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} a_c^k(t), \tag{A1}$$

with a similar equation for $\tilde{f}_b^j$. The Fourier transformed version of Eq. (2) is

$$[-i\omega\delta^{jk}\delta_{bc} + G_{bc}^{jk}]a_c^k(\omega) = \tilde{f}_b^j(\omega). \tag{A2}$$

If we define

$$(\mathcal{G}^{-1})_{bc}^{jk}(\omega) = [-i\omega\delta^{jk}\delta_{bc} + G_{bc}^{jk}], \tag{A3}$$

then Eq. (A2) has the form $(\mathcal{G}^{-1})_{bc}^{jk}(\omega)a_c^k(\omega)=\tilde{f}_b^j(\omega)$. It then follows from Eq. (4) that

$$\mathcal{P}[\underline{\boldsymbol{f}}] \sim \exp -\frac{1}{4}\int \frac{d\omega}{2\pi}\tilde{f}_b^j(-\omega)(Q^{-1})_{bc}^{jk}\tilde{f}_c^{\,k}(\omega)$$

$$\Rightarrow P[\underline{\boldsymbol{a}}] \sim \exp -\frac{1}{4}\int \frac{d\omega}{2\pi} a_b^j(-\omega)(\mathcal{G}^{T-1}(-\omega)Q^{-1} \times \mathcal{G}^{-1}(\omega))_{bc}^{jk} a_c^k(\omega),$$

which is Eq. (6) where the matrix $B(\omega)$ is given by $B(\omega) = \mathcal{G}(\omega)Q\mathcal{G}^T(-\omega)$. From Eq. (A3), $\mathcal{G}^*(\omega)=\mathcal{G}(-\omega)$, and therefore $\mathcal{G}^T(-\omega)=\mathcal{G}^\dagger(\omega)$, and so another form for $B(\omega)$ is Eq. (7).

Next we wish to show that the result (11) for the correlation function, and the response function (14), may be found by averaging $a_b^j(\omega)a_c^k(-\omega)$ and $a_b^j(\omega)\hat{a}_c^k(-\omega)$, respectively, with a weight given by the exponential in Eq. (17).

The functional integrals which we wish to evaluate are of the form

$$\int \left(\prod_{b=1}^{N} D\boldsymbol{a}_b D\hat{\boldsymbol{a}}_b\right) f(\boldsymbol{a}_c(\omega),\hat{\boldsymbol{a}}_d(\omega))P[\underline{\boldsymbol{a}},\underline{\hat{\boldsymbol{a}}}], \tag{A4}$$

where

$$P[\underline{\boldsymbol{a}},\underline{\hat{\boldsymbol{a}}}] = \exp\int \frac{d\omega}{2\pi}[i\hat{a}_b^j(-\omega)(\mathcal{G}^{-1})_{bc}^{jk}(\omega)a_c^k(\omega) - \hat{a}_b^j(-\omega)Q_{bc}^{jk}\hat{a}_c^k(\omega)], \tag{A5}$$

as in Eq. (17) and where $f(\boldsymbol{a}_c(\omega),\hat{\boldsymbol{a}}_d(\omega))$ is equal to $a_b^j(\omega)\hat{a}_c^k(-\omega)$ in the case of the numerator of the response function, to $a_b^j(\omega)a_c^k(-\omega)$ for the numerator of the correlation function, and to 1 for denominator of both the response function and the correlation function.

If we make the change of variable $\hat{a}_c'^{k}(\omega) = \hat{a}_b^j(\omega)(\mathcal{G}^{-1})_{bc}^{jk}(-\omega)$, used to obtain Eq. (18) from Eq. (17) in Sec. II, the expression for the correlation function is unchanged, since a common factor cancels between the numerator and denominator, but the response function is multiplied by the matrix $\mathcal{G}(\omega)$. Going back to the time variable, we may write the integrals we now have to perform in the form

$$\int d\boldsymbol{y}\int \frac{d\boldsymbol{x}}{(2\pi)^n}g(\boldsymbol{x},\boldsymbol{y})e^{i\boldsymbol{x}\cdot\boldsymbol{y}-\boldsymbol{x}\cdot\boldsymbol{B}\cdot\boldsymbol{x}}. \tag{A6}$$

Here we have now discretized time as well as space, and the time, space and internal $(b=1,\ldots,N)$ labels will all be incorporated into a single index $(I,J=1,\ldots,n)$. Thus the integrals in Eq. (A6) are n-fold integrals, and $\boldsymbol{x}$ and $\boldsymbol{y}$ are n-component vectors. The function $g(\boldsymbol{x},\boldsymbol{y})$ is $x_I y_J$ for the numerator of response function, $y_I y_J$ for numerator of the correlation function, and 1 for the denominator. Note that we have omitted the Jacobian factor, and all other constant factors, since they cancel when averages are being calculated.

All the above hold whether or not the matrix Q, and hence the matrix B, is singular. We wish to evaluate Eq. (A6) without making the assumption that Q or B are nonsingular. To do this when $g=1$ is straightforward, since the y integrations give a product of n delta-functions with arguments which are the components of $\boldsymbol{x}$ and also n factors of 2π which cancel the $(2\pi)^n$. Therefore the final integrals over the x variables give 1. This means that the denominator in any average is equal to unity, and may be omitted from now on. When $g = x_I y_J$, we may carry out the y integrations in a similar manner to give

$$-i\int d\boldsymbol{x}\left\{\frac{\partial}{\partial x_J}\delta(\boldsymbol{x})\right\}x_I e^{-\boldsymbol{x}\cdot\boldsymbol{B}\cdot\boldsymbol{x}}, \tag{A7}$$

which gives $i\delta_{IJ}$ after integration by parts. Finally, when $g = y_I y_J$, we find

$$-\int d\boldsymbol{x}\left\{\frac{\partial^2}{\partial x_I\,\partial x_J}\delta(\boldsymbol{x})\right\}e^{-\boldsymbol{x}\cdot\boldsymbol{B}\cdot\boldsymbol{x}} = 2B_{IJ}. \tag{A8}$$

We should stress again that these results have been derived without making the assumption that Q, and so B, is nonsingular. So, in summary, we have

$$\langle a_b^j(\omega)\hat{a}_c^k(-\omega)\rangle = i\mathcal{G}_{bc}^{\,jk}(\omega) \tag{A9}$$

and

$$\langle a_b^j(\omega)a_c^k(-\omega)\rangle = 2B_{bc}^{jk}(\omega). \tag{A10}$$

APPENDIX B: INVERSION OF THE MATRIX $\mathcal{G}^{-1}$

From Eq. (47) we have that

$$\mathcal{G}^{-1}(\boldsymbol{k},\omega) = \begin{pmatrix} r_0k^2 & ir_1k_\mu & 0 \\ ir_1k_\mu & r_3k_\mu k_\nu - r_4k^2\delta_{\mu\nu} & ir_2k_\mu \\ 0 & ir_2k_\mu & r_5k^2 \end{pmatrix}, \tag{B1}$$

where the constants $r_0,r_1,\ldots,r_5$ are given by

$$r_0 = -i\omega', \quad r_1 = c_1,$$

$$r_2 = c_2, \quad r_3 = c_3,$$

$$r_4 = +i\omega' + c_4, \quad r_5 = -i\omega' + c_5. \tag{B2}$$

Here $\omega' = \omega/k^2$ and the constants $c_1,\ldots,c_5$ are given by Eq. (48).

From the symmetry properties of the system, we expect that the inverse of Eq. (B1) will have the form

$$\mathcal{G}(\boldsymbol{k},\omega)=\begin{pmatrix} s_0 & is_1k_\mu & s_6 \\ is_1k_\mu & s_3k_\mu k_\nu - s_4k^2\delta_{\mu\nu} & is_2k_\mu \\ s_6 & is_2k_\mu & s_5 \end{pmatrix}, \qquad \text{(B3)}$$

where the constants $s_0, s_1, \ldots, s_6$ are to be determined in terms of the constants $r_0, r_1, \ldots, r_5$.

By direct multiplication of Eqs. (B1) and (B3) we can verify that $\mathcal{G}(\boldsymbol{k},\omega)$ does indeed have the form given by Eq. (B3), and that the constants $s_0, s_1, \ldots, s_6$ are given by

$$r_0s_0k^2 - r_1s_1k^2 = 1,$$

$$r_1s_0 + (r_3 - r_4)s_1k^2 + r_2s_6 = 0,$$

$$-r_2s_1 + r_5s_6 = 0, \qquad \text{(B4)}$$

$$r_4s_4(k^2)^2 = 1,$$

$$r_0s_1 + r_1(s_3 - s_4) = 0,$$

$$r_1s_1 - (r_3 - r_4)s_3k^2 + r_3s_4k^2 + r_2s_2 = 0,$$

$$r_2(s_3 - s_4) + r_5s_2 = 0, \qquad \text{(B5)}$$

and

$$r_0s_6 - r_1s_2 = 0,$$

$$r_1s_6 + (r_3 - r_4)s_2k^2 + r_2s_5 = 0,$$

$$-r_2s_2k^2 + r_5s_5k^2 = 1. \qquad \text{(B6)}$$

This set of 10 equations reduce to

$$s_1 = -\frac{r_1r_5}{D}s_0, \quad s_2 = -\frac{r_0r_2}{D}s_0,$$

$$s_4 - s_3 = -\frac{r_0r_5}{D}s_0, \quad s_6 = -\frac{r_1r_2}{D}s_0, \qquad \text{(B7)}$$

with

$$k^2(r_0s_0 - r_1s_1) = 1, \quad (k^2)^2r_4s_4 = 1,$$

$$k^2(r_5s_5 - r_2s_2) = 1, \qquad \text{(B8)}$$

where $D = r_2^2 + (r_3 - r_4)r_5k^2$. From Eqs. (B7) and (B8) any of the $s_0, s_1, \ldots, s_6$ can be easily determined.

In Sec. IV we discuss an example for which we only need to find s_0. From the first equations of Eqs. (B7) and (B8) we find this is given by

$$k^2s_0 = \frac{r_2^2 + (r_3 - r_4)r_5k^2}{(r_0r_2^2 + r_5r_1^2) + r_0(r_3 - r_4)r_5k^2}. \qquad \text{(B9)}$$

Writing this in terms of the physical constants defined by Eq. (48) results in the expression for $s_0 (= \mathcal{G}_{11}(\boldsymbol{k},\omega))$ given by Eq. (51) of Sec. IV.

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