Large deviations of heat flow in harmonic chains

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Abstract. We consider heat transport across a harmonic chain connected at its two ends to white-noise Langevin reservoirs at different temperatures. In the steady state of this system the heat $Q$ flowing from one reservoir into the system in a finite time $\tau$ has a distribution $P(Q, \tau)$. We study the large time form of the corresponding moment generating function $\langle e^{-\lambda Q} \rangle \sim g(\lambda)e^{\tau \mu(\lambda)}$. Exact formal expressions, in terms of phonon Green’s functions, are obtained for both $\mu(\lambda)$ and also the lowest order correction $g(\lambda)$. We point out that, in general, a knowledge of both $\mu(\lambda)$ and $g(\lambda)$ is required for finding the large deviation function associated with $P(Q, \tau)$. The function $\mu(\lambda)$ is known to be the largest eigenvector of an appropriate Fokker–Planck type operator and our method also gives the corresponding eigenvector exactly.

Keywords: current fluctuations, large deviations in non-equilibrium systems, heat conduction

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1. Introduction

Among the most interesting recent developments in the theory of nonequilibrium processes are the so-called fluctuation theorems \cite{1}–\cite{7}. These theorems make quantitative statements on the probability of negative entropy production in nonequilibrium systems. They have been theoretically \cite{8}–\cite{19} and experimentally \cite{20}–\cite{28} studied in a large number of systems in various nonequilibrium states. The results have been obtained in the contexts of both transient and steady state phenomena. In the case of nonequilibrium steady states in systems carrying heat or particle currents, the fluctuation theorems have pointed to the importance of the large deviation function (LDF) and the cumulant generating function (CGF) \cite{29}. The steady state fluctuation theorem can, in these cases, be equivalently stated as a symmetry property of the LDF or the CGF \cite{12,14,15}. Apart from their interest from the viewpoint of the fluctuation theorem, these two functions contain important information on nonequilibrium processes: the LDF gives the precise probability of the occurrence of rare events while the CGF contains information on the average current in a system as well as all moments \cite{29}. So far there have been very few examples where either the LDF or the CGF has been exactly computed. The few examples include particle transport in exclusion processes \cite{12,14,15}, Brownian motors \cite{18,19}, power dissipation and heat transport in single Brownian particles \cite{16}, \cite{30}–\cite{32} and heat conduction across a quantum harmonic chain \cite{17}.

Consider the example of heat conduction through a system coupled to two heat baths at different temperatures $T_L$ and $T_R$ and let $Q$ be the heat flowing from the left reservoir into the system during a time interval $\tau$. Then $Q$ is a stochastic variable with a distribution $P(Q)$ and the LDF and CGF for this problem are defined by the following scaling forms,
valid for large $\tau$:
\[ P(Q, \tau) \sim e^{-\tau h(Q/\tau)} \]
\[ Z(\lambda) = \langle e^{-\lambda Q} \rangle = \int_{-\infty}^{\infty} dQ e^{-\lambda Q} P(Q, \tau) \sim g(\lambda)e^{\tau \mu(\lambda)}. \]

We will refer to $h(q)$ and $\mu(\lambda)$ as the LDF and CGF respectively. For large $\tau$ the term $g(\lambda)$ is a correction to the CGF and can normally be ignored in the saddle-point calculation which relates $h(q)$ and $\mu(\lambda)$. The saddle-point calculation gives
\[ h(q) = -[\mu(\lambda^*) + q\lambda^*], \quad \mu'(\lambda^*) = -q. \]

While the LDF and the CGF are normally related by Legendre transformations, there are several examples where this relation is known to break down. This happens if the function $g(\lambda)$ has singularities in the region of the saddle-point integration. Interestingly, in such cases, the CGF might still satisfy the fluctuation symmetry relation, while the LDF does not [16, 32, 33]. Thus we note that if one is interested in the LDF then it is in general important to calculate both $\mu(\lambda)$ and the leading correction term $g(\lambda)$. Of course $\mu(\lambda)$ is itself of interest since it contains important information on current and current-noise properties and relations between response functions.

The aim of this paper is to present a formalism for obtaining $\mu(\lambda)$ as well as $g(\lambda)$ for the problem of heat conduction across a harmonic chain connected to white-noise Langevin heat baths. We use the linearity of the problem and show that the problem of finding the generating function $Z(\lambda)$ reduces to performing multi-dimensional Gaussian integrations. We are able to find a closed form expression for $\mu(\lambda)$, as given by (11), in terms of the phonon transmission function, a well known quantity in the study of heat conduction in harmonic systems. Finding $g(\lambda)$ is more difficult but we are able to also express it, as given by (59), in terms of appropriate phonon Green’s functions. For the case of a single free Brownian particle we can use our approach to explicitly obtain both $\mu(\lambda)$ and $g(\lambda)$ and for this case we recover the results of Visco [16], obtained by solving the Fokker–Planck equation.

The paper is organized as follows. In section 2 we define the model that we study, make some general remarks on the problem of computing the generating function for heat, and briefly explain our method. In section 3 we give the calculation of the CGF $\mu(\lambda)$ while in section 4 we give the calculation of the correction term $g(\lambda)$. The example of a single Brownian particle, for which explicit results for $\mu(\lambda)$ and $g(\lambda)$ can be obtained, are considered in section 5. Finally we discuss our results in section 6.

### 2. The model and general considerations

We consider a one-dimensional chain of $N$ particles with harmonic interactions and described by the Hamiltonian
\[ \mathcal{H} = \sum_{l=1}^{N} \frac{1}{2} m_l v_l^2 + \frac{1}{2} \sum_{l=1}^{N} \sum_{m=1}^{N} \Phi_{lm} x_l x_m, \]
where $x_l$, $v_l$ and $m_l$ are, respectively, the displacement about the equilibrium position, velocity and mass of the $l$th particle and the matrix $\Phi$ represents the force matrix of
the system. For the moment we assume that at least one site of the chain is pinned such that the centre of mass attains a steady state distribution. However, later we show that the results are also valid for a free harmonic chain. The particles 1 and $N$ at the two ends—which we refer to as left (L) and right (R) respectively—are coupled to white-noise Langevin heat reservoirs at two different temperatures $T_L$ and $T_R$ respectively. The system, described by the variables $X^T = (x_1, x_2, \ldots, x_N)$ and $V^T = (v_1, v_2, \ldots, v_N)$, evolves according to the following equations of motion:

$$
X = V, \quad M \dot{V} = -\Phi X - \gamma V + \eta(t),
$$

where $M = \text{diag}(m_1, m_2, \ldots, m_N)$ is the mass matrix, the dissipation matrix $\gamma$ has matrix elements $\gamma_{i,j} = \delta_{i,j}(\delta_{i,1} \gamma_L + \delta_{i,N} \gamma_R)$ and the noise vector $\eta$ has elements $\eta_i(t) = \delta_{i,1} \eta_L(t) + \delta_{i,N} \eta_R(t)$. The variables $\eta_L(t), \eta_R(t)$ are zero-mean Gaussian white noises with correlations given by

$$
\langle \eta_\alpha(t) \eta_{\alpha'}(t') \rangle = 2 \delta_{\alpha,\alpha'} d_\alpha \delta(t - t'), \quad \text{where } d_\alpha = \gamma_\alpha T_\alpha, \quad \alpha, \alpha' = \text{L, R}
$$

and we have set the Boltzmann constant $k_B = 1$.

Since the equations of motion (4) are linear and the noise vector $\eta$ is Gaussian, the probability distribution function of the phase space variables $U^T = (X^T, V^T)$ in the nonequilibrium steady state is a Gaussian with mean $\langle U \rangle = 0$ and with covariance matrix $\lim_{t \to \infty} \langle U(t) U^T(t) \rangle$. We denote the nonequilibrium steady state distribution by $P_{\text{SS}}(U)$. The covariance matrix of the ordered harmonic chain was obtained exactly in [34]. For mass-disordered systems the covariance matrix can be expressed in terms of phonon Green’s functions [35, 36]. The quantity of interest to us here is the total amount of heat, $Q$, flowing from one of the reservoirs—say the left (L)—into the system in a given time duration $\tau$, in the nonequilibrium steady state. This is given by

$$
Q = \int_0^\tau [\eta_L(t) - \gamma_L v_1(t)] v_1(t) \, dt,
$$

where $v_1(t)$ evolves according to (4), with the initial condition at $t = 0$ drawn from the nonequilibrium steady state distribution. Clearly, $Q$ is a fluctuating quantity whose value depends on the initial conditions $U_0 = U(t = 0)$ and the noise trajectory $\{\eta(t); 0 \leq t \leq \tau\}$ during any particular realization. Let $P(Q, \tau)$ denote the probability distribution of $Q$ and let $Z(\lambda) = \langle e^{-\lambda Q} \rangle$ be the corresponding characteristic function, where $\langle \cdots \rangle$ denotes an average over initial configurations as well as over different paths.

It is useful to consider the restricted characteristic function $Z(\lambda, U, \tau|U_0) = \langle e^{-\lambda Q} \rangle_{U_0,U}$. As shown in appendix A, this satisfies a Fokker–Planck type equation:

$$
\partial_t Z(\lambda, U, \tau|U_0) = \mathcal{L}_\lambda Z(\lambda, U, \tau|U_0),
$$

with the initial condition $Z(\lambda, U, 0|U_0) = \delta(U - U_0)$. The solution of this can formally be written down in the eigenbases of the Fokker–Planck operator $\mathcal{L}_\lambda$, and the large $\tau$ behaviour is dominated by the term having the largest eigenvalue $\mu(\lambda)$, i.e.,

$$
Z(\lambda, U, \tau|U_0) \sim \chi(U_0, \lambda) \Psi(U, \lambda) \exp[\tau \mu(\lambda)]
$$

where $\Psi(U, \lambda)$ is the eigenfunction corresponding to the largest eigenvalue, i.e., $\mathcal{L}_\lambda \Psi(U, \lambda) = \mu(\lambda) \Psi(U, \lambda)$, and $\chi(U_0, \lambda)$ is the projection of the initial state onto the
eigenstate corresponding to the eigenvalue $\mu(\lambda)$. We note that for $\lambda = 0$, $Z(\lambda = 0, U, \tau|U_0)$ is just the phase space distribution at time $\tau$. Hence the existence of a unique nonequilibrium steady state, which has been proved for this system [36], requires that $Z(\lambda = 0, U, \tau \rightarrow \infty|U_0) = P_{SS}(U)$, and this implies that $\mu(0) = 0$, $\chi(U_0, 0) = 1$ and $\Psi(U, 0) = P_{SS}(U)$. Using (8), and the fact that $P_{SS}(U) = \Psi(U, 0)$, we get for large $\tau$

$$Z(\lambda) = \int dU_0 \int dU \, \Psi(U_0, 0) Z(\lambda, U, \tau|U_0) \sim g(\lambda) \exp[\tau \mu(\lambda)],$$

where $g(\lambda) = \int dU_0 \, \Psi(U_0, 0) \chi(U_0, \lambda) \int dU \, \Psi(U, \lambda)$. (9)

Note that $g(0) = 1$. As discussed in section 1 the large deviation function $h(q = Q/\tau) = -\lim_{\tau \rightarrow \infty} \ln P(Q, \tau)/\tau$ is given by the Legendre transformation

$$h(q) = -[\mu(\lambda^*) + \lambda^* q],$$

with $\lambda^*(q)$ implicitly given by the saddle-point equation $\mu'(\lambda^*) = -q$. The above relation holds provided that $g(\lambda)$ is analytic along the real $\lambda$ in the region $[0, \lambda^*]$, and so $g(\lambda)$ can be neglected in the saddle-point calculation as a subleading contribution and the contour of integration can be deformed smoothly through the saddle-point $\lambda^*$. On the other hand, if $g(\lambda)$ possesses any singularity in the region $[0, \lambda^*]$, then the contour of the integration cannot be deformed smoothly through the saddle-point $\lambda^*$, and one needs to include $g(\lambda)$ in the saddle-point calculation.

The calculation of the LDF thus requires one to compute the CGF $\mu(\lambda)$ and the leading correction $g(\lambda)$. From the above discussion we see that these can be obtained from the largest eigenvalue and eigenvector of an appropriate Fokker–Planck operator for this system. This is however very difficult in most cases, including for the model studied here. However the linearity of the dynamics and the Gaussian nature of the noise in the present problem allow the computation of $\mu(\lambda)$ and $g(\lambda)$ using a different approach. The basic idea that we use is that the variable of interest $Q$ is a quadratic function of the initial phase space configuration $U_0$ and the noise trajectories $\{\eta(t): 0 \leq t \leq \tau\}$, both of which are Gaussian distributed variables. Hence the problem of computing $\langle e^{-\lambda Q}\rangle$ reduces to that of doing a multi-variate Gaussian integration. In the following sections we present the details.

We make some remarks on the symmetry property of the CGF. In general, if the operator $L_{\lambda}$ and its adjoint $L_{\lambda}^\dagger$ possess the symmetry $L_{\lambda}^\dagger = L_{a-\lambda}$, then it immediately follows that $\mu(\lambda) = \mu(a-\lambda)$. Even if another operator $L_{\lambda}^\prime$—which is related to $L_{\lambda}$ by a similarity transformation—possesses the symmetry $L_{\lambda}^\dagger = L_{a-\lambda}^\prime$, then $\mu(\lambda)$ also has the above symmetry. There are some examples of systems with Markovian dynamics where the evolution operator satisfies this property but this does not seem to be the case for the model discussed here. In fact, even for the simplest case of a single free Brownian particle connected to two heat reservoirs [16], the Fokker–Planck operator does not possesses the above mentioned symmetry. In this case however, the Fokker–Planck operator can be transformed to a Hermitian operator of a quantum harmonic oscillator where the potential remains invariant under $\lambda \rightarrow (\Delta \beta - \lambda)$. We are not aware of such a transformation for a system having more than one particle and hence the symmetry of $\mu(\lambda)$ is a non-trivial one.
3. Calculation of the CGF $\mu(\lambda)$

Before giving the details of the calculation we first state our main result of this section for the CGF, which is

$$\mu(\lambda) = -\frac{1}{4\pi} \int_{-\infty}^{\infty} d\omega \ln[1 + T(\omega)T_L T_R \lambda(\Delta\beta - \lambda)],$$  \hspace{1cm} (11)

where $\Delta\beta = T_R^{-1} - T_L^{-1}$ and

$$T(\omega) = 4\gamma_L \gamma_R \omega^2 G_{1,N}^+(\omega)G_{1,N}^-(\omega),$$  \hspace{1cm} (12)

with $G^\pm(\omega) = [\Phi - \omega^2 M \pm i\omega\gamma]^{-1}$. \hspace{1cm} (13)

Note that $G^-(\omega) = G^+(\omega)$ and the Green’s function matrix $G^+(\omega)$ is given by (13). Since $\tilde{\eta} \sim 1/\tau^{1/2}$ and $\Delta X_\tau, \Delta V_\tau$ have finite variances for large $\tau$, it follows that the second term in (17) is $O(1/\tau^{1/2})$ smaller.

We now give the details of the derivation of the expression (11). We solve the Langevin equations of motion by using Fourier transforms. Let us define the finite-time Fourier transform of (4) gives the velocity vector in the frequency domain as

$$\tilde{V}(\omega) = i\omega G^\dagger \tilde{\eta} + \frac{1}{\tau} G^\dagger (\Phi \Delta X_\tau - i\omega M \Delta V_\tau),$$  \hspace{1cm} (17)

where $\Delta X_\tau = X(\tau) - X(0)$, $\Delta V_\tau = V(\tau) - V(0)$, and the Green’s function matrix $G^+(\omega)$ is given by (13). Since $\tilde{\eta} \sim 1/\tau^{1/2}$ and $\Delta X_\tau, \Delta V_\tau$ have finite variances for large $\tau$, it follows that the second term in (17) is $O(1/\tau^{1/2})$ smaller.

Taking the Fourier transform of (4) gives the velocity vector in the frequency domain as

$$\tilde{V}(\omega) = i\omega G^\dagger \tilde{\eta} + \frac{1}{\tau} G^\dagger (\Phi \Delta X_\tau - i\omega M \Delta V_\tau),$$  \hspace{1cm} (17)

and the Green’s function matrix $G^+(\omega)$ is given by (13). Since $\tilde{\eta} \sim 1/\tau^{1/2}$ and $\Delta X_\tau, \Delta V_\tau$ have finite variances for large $\tau$, it follows that the second term in (17) is $O(1/\tau^{1/2})$ smaller.

The Gaussian noise configurations represented by $\{\eta(t) : 0 < t < \tau\}$ can now equivalently be described in the frequency domain, by the infinite sequence $\{\tilde{\eta}(\omega_n) : n = -\infty, \ldots, -1, 0, \ldots, \infty\}$ of Gaussian random variables having the correlations

$$\langle \tilde{\eta}_\alpha(\omega) \tilde{\eta}_{\alpha'}(\omega') \rangle = 2\delta_{\alpha,\alpha'} \frac{\gamma_\alpha \tau}{\tau} \delta[\omega + \omega'], \hspace{1cm} \text{with } \alpha, \alpha' = L, R.$$  \hspace{1cm} (16)

Henceforth for convenience we will drop the subscript $n$ from $\omega_n$. Taking the Fourier transform of (4) gives the velocity vector in the frequency domain as

$$\tilde{V}(\omega) = i\omega G^\dagger \tilde{\eta} + \frac{1}{\tau} G^\dagger (\Phi \Delta X_\tau - i\omega M \Delta V_\tau),$$  \hspace{1cm} (17)

and the Green’s function matrix $G^+(\omega)$ is given by (13). Since $\tilde{\eta} \sim 1/\tau^{1/2}$ and $\Delta X_\tau, \Delta V_\tau$ have finite variances for large $\tau$, it follows that the second term in (17) is $O(1/\tau^{1/2})$ smaller.

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In terms of the Fourier transform, the expression in (6) for the heat transfer becomes

\[ \tilde{v}_1(\omega) \sim i \omega [G_{-1}^T(\omega) \tilde{\eta}_L(\omega) + G_{-N}^T(\omega) \tilde{\eta}_R(\omega)]. \]  

(18)

In terms of the Fourier transform, the expression in (6) for the heat transfer becomes

\[ Q(\tau) = \tau \sum_{n=-\infty}^{\infty} \tilde{q}_n \quad \text{with} \quad \tilde{q}_n = \tilde{\eta}_L(\omega) \tilde{v}_1(-\omega) - \gamma_L \tilde{v}_1(\omega) \tilde{v}_1(-\omega). \]  

(19)

For a chain with at least one pinned site it is easily seen from (18) that \( \tilde{v}_1(0) = 0 \) and hence the heat transfer \( \tilde{q}_0 \) through the zeroth mode vanishes in (19). This is related to the fact that for a pinned system there is no zero-frequency mode available for transporting energy. Substituting (18) in (19) we write \( Q(\tau) = \tau \sum_{n=1}^{\infty} (\tilde{q}_n + \tilde{q}_{-n}) \) and using the fact \( \tilde{\eta}_n(-\omega) = \tilde{\eta}^*_{-n}(\omega) \) we get

\[ Z(\lambda) = \langle e^{-\lambda Q} \rangle \sim \prod_{n=1}^{\infty} \langle e^{-\frac{\lambda}{2} \xi_n^T A_n \xi_n^*} \rangle, \quad \text{where} \quad \xi_n = (\tilde{\eta}_L(\omega), \tilde{\eta}_R(\omega))^T, \]  

(20)

and

\[ A_n = \begin{pmatrix} 2\gamma_R \omega^2 |G_{1,n}^T|^2 & -i\omega G_{-1,n}^- - 2\gamma_L \omega^2 G_{1,n}^+ G_{1,n}^- \\ i\omega G_{1,n}^- - 2\gamma_L \omega^2 G_{1,n}^+ G_{1,n}^- & -2\gamma_L \omega^2 |G_{1,n}^+|^2 \end{pmatrix}, \]  

(21)

where in obtaining the (1,1)th element above we have made use of the identity

\[ -\text{Im} G_{1,1}^+(\omega) = \omega [\gamma_L |G_{1,1}^+(\omega)|^2 + \gamma_R |G_{1,n}^+(\omega)|^2], \]  

(22)

which can be proved as follows. From the definition of the Green’s function in (13) we have \( [G^+]^{-1} - [G^-]^{-1} = 2i\omega \gamma \). Multiplying both sides by \( G^+ \) from the left and by \( G^- \) from the right we get \( G^- G^+ = 2i\omega G^+ G^- \). The (1,1)th element of this leads to (22). For each \( n \), the average in (20) is evaluated with respect to the Gaussian distribution

\[ p(\xi_n) = \frac{1}{\pi^d |\text{det} D|} \exp \left( -\xi_n^T D^{-1} \xi_n \right), \quad \text{with} \quad D = \text{diag} \left( \frac{2dL}{\tau}, \frac{2dR}{\tau} \right). \]  

(23)

Hence we get (see appendix B)

\[ \langle e^{-\lambda T \xi_n^T A_n \xi_n^*} \rangle = [\text{det} (I + \lambda T D A_n)]^{-1}, \]  

(24)

\[ = [1 + T(\omega)T_L T_R \lambda (\Delta \beta) - \lambda]^{-1}, \]  

(25)

where \( T(\omega) \) is given by (12). Using (20) and (25) and noting that in the \( \tau \to \infty \) limit we can replace the summation over \( n \) by an integral over \( \omega \) we obtain our final result in (11).

We remark that the result (11) is in fact valid for both pinned as well as unpinned cases. For the unpinned harmonic system the centre of mass coordinate does not reach a steady state and it is useful to separate out this degree of freedom. Let us define new relative coordinates \( y_l = x_l - x_{N}, l = 1, 2, \ldots, N - 1 \). The facts that the unpinned system has translational symmetry and that \( \Phi \) is a symmetric matrix imply the relation

\[ \sum_{l=1,N} \Phi_{l,j} = \sum_{j=1,N} \Phi_{l,j} = 0. \]  

Using this we get from (4)

\[ \dot{y}_l = v_l - v_{N}, \quad l = 1, 2, \ldots, N - 1 \]  

(26)

\[ m_l \ddot{v}_l = -\sum_{j=1}^{N-1} \Phi_{l,j} y_j - \gamma_l \dot{v}_l + \eta(t), \quad l = 1, 2, \ldots, N. \]  

(27)
The relative coordinates \( y_l, l = 1, 2, \ldots, N - 1 \) attain the steady state with finite variance and it follows then from (26) that \( \tilde{v}_l(\omega = 0) \sim \tilde{v}_N(\omega = 0) \) up to order \( O(1/\tau) \). Then from (27) we get \( \tilde{v}_l(0) \sim [\tilde{\eta}_l(0) + \tilde{\eta}_R(0)]/[(\gamma_L + \gamma_R)] \) for all \( l \). We use this to compute the \( \tilde{q}_0 \neq 0 \) term in (19). With \( \xi_0 = (\tilde{\eta}_L(0), \tilde{\eta}_R(0))^T \), we get

\[
\tilde{q}_0 \sim \frac{1}{2} \xi_0^T A_0 \xi_0 \quad \text{where} \quad A_0 = \begin{pmatrix}
2\gamma_R & (\gamma_L + \gamma_R)^2 & -\gamma_L - \gamma_R \\
(\gamma_L + \gamma_R)^2 & -\gamma_L - \gamma_R & (\gamma_L + \gamma_R)^2 \\
(\gamma_L + \gamma_R)^2 & (\gamma_L + \gamma_R)^2 & 2\gamma_L
\end{pmatrix}.
\]  

(28)

The noise \( \xi_0 \) has the Gaussian distribution

\[
p(\xi_0) = \frac{1}{2\pi \sqrt{\det D}} \exp \left( -\frac{1}{2} \xi_0^T D^{-1} \xi_0 \right)
\]  

(29)

and hence we get

\[
\langle e^{-\lambda \tilde{q}_0} \rangle \sim [\det(\Psi + \lambda \tau DA_0)]^{-1/2} = [1 + \mathcal{T}(0)T_L T_R \lambda (\Delta \beta - \lambda)]^{-1/2}
\]  

(30)

where \( \mathcal{T}(0) = 4\gamma_L \gamma_R / (\gamma_L + \gamma_R)^2 \) is precisely what one obtains by taking \( \mathcal{T}(\omega \rightarrow 0) \) in (12) for the unpinned system. This follows from the fact that in this case \( G_{1N}^+ / \omega \sim 1/\omega (\gamma_L + \gamma_R) \), a result which we now prove. For any matrix \( A \) let \( A_{(i,j)}^{(k,l)} \) denote the submatrix of \( A \) that occurs between the \((i,j)\)th and the \((k,l)\)th elements. Also let \( B = -M \omega^2 + \Phi + i\omega \gamma \). Then we have \( G_{1N}^+ = (-1)^{N+1} \det B_{(N-1,N)}^{(1,2)}/\det B \) Taylor expanding the determinants about \( \omega = 0 \) we obtain \( \det B_{(N-1,N)}^{(1,2)} = \det \Phi_{(N-1,N)} \) and \( \det B_{1N} = i\omega \gamma L \det \Phi_{(1,1)}^{(2,2)} \). For the \( N \)-1 case, we have used \( \det B = \det \Phi_{(1,1)}^{(2,2)} \) that follows from the property \( \sum_{i=1,N-1} \Phi_{i,j} = \sum_{j=1,N} \Phi_{i,j} = 0 \). Using the latter property it is easy to show that \( \det \Phi_{(1,1)}^{(2,2)} = \det \Phi_{(1,1)}^{(2,2)} = (-1)^{N-1} \det \Phi_{(1,1)}^{(2,2)} \). Hence we get the desired result.

4. Calculation of \( g(\lambda) \)

We turn now to the more difficult problem of calculating \( g(\lambda) \) which requires one to keep the second term in (17) and perform the averaging over initial conditions, in addition to the noise averaging. We recall that the heat transfer is given by (19) where the velocity \( \tilde{v}_1 \) can be obtained from the following exact solution for \( X, \hat{V} \):

\[
\hat{X} = G^+ \tilde{\eta} - \frac{1}{\tau} G^+(i\omega M \Delta X + \gamma \Delta X + M \Delta V),
\]

\[
\hat{V} = i\omega G^+ \tilde{\eta} + \frac{1}{\tau} G^+(\Phi \Delta X - i\omega M \Delta V),
\]  

(31)

where \( \Delta X = X(\tau) - X(0), \quad \Delta V = V(\tau) - V(0) \).

To obtain \( Z(\lambda) = \langle e^{-\lambda \tilde{q}} \rangle \) we need to average over both the noise \( \tilde{\eta} \) and the initial steady state distribution of \( U_0 \). We note that the solution in (31) contains \( U^T(\tau) = (X^T(\tau), V^T(\tau)) \) and this has to be expressed in terms of \( \tilde{\eta} \) and \( U_0 \). While this can be done, we follow a different strategy which is more convenient.

It is easier to calculate the restricted generating function

\[
Z(\lambda, U, \tau | U_0) = \langle e^{-\lambda \tilde{q}} \delta(U - U(\tau)) \rangle_{U_0},
\]  

(32)

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where the average is performed only over noise and for a given initial condition $U_0$. We can then obtain $Z(\lambda) = \int dU \int dU_0 P_\lambda(U_0) Z(\lambda, U, \tau|U_0)$. The steps of the calculation now are as follows. We first note that, because of the $\delta$-function constraint in (32), we can obtain $Q$ as a quadratic function of the variables $\tilde{\eta}, U, U_0$. This follows from (19) by using the following expression for $\tilde{\eta}$, obtained from (31) by replacing $U(\tau)$ by $U$:

$$
\tilde{\eta}(\omega) = i\omega [G_{11i}^+ \tilde{\eta}_L + G_{1N}^+ \tilde{\eta}_R] + \frac{1}{\tau} \sum_{l=1,N} [(G^+\Phi)_{ll} \Delta X_l - i\omega(G^+M)_{ll} \Delta V_l]
$$

$$
= i\omega [G_{11i}^+ \tilde{\eta}_L + G_{1N}^+ \tilde{\eta}_R] + \frac{1}{\tau} F_1^T \Delta U,
$$

where

$$
\Delta X = X - X(0), \quad \Delta V = V - V(0), \quad \Delta U = U - U(0), \quad \text{and}
$$

$$
F_1^T = ((G^+\Phi)_{1,1}, (G^+\Phi)_{1,2}, \ldots, (G^+\Phi)_{1,N}, -i\omega[G^+M]_{1,1}, -i\omega[G^+M]_{1,2}, \ldots, -i\omega[G^+M]_{1,N}).
$$

We replace the $\delta$-function in (32) by the integral representations $\delta(U - U(\tau)) = \int d^{2N}\sigma/(2\pi)^{2N} e^{i\sigma^T(U - U(\tau))}$ where $\sigma^T = (\sigma_1, \sigma_2, \ldots, \sigma_{2N})$. We then have

$$
Z(\lambda, U, \tau|U_0) = \int \frac{d^{2N}\sigma}{(2\pi)^{2N}} e^{i\sigma^T U} \langle e^{E(\tau)} \rangle_{U=U_0}
$$

(35)

where $E(\tau) = -\lambda Q - i\sigma^T U(\tau)$.

We need an expression for $U^T(\tau) = (X^T(\tau), V^T(\tau))$ which we now obtain. We note that since we are using a Fourier series representation for $X(t), V(t)$, the correct value at time $\tau$ is obtained from the Fourier series by setting $t = \tau - \epsilon, \epsilon > 0$ and taking the limit $\epsilon \to 0$. Hence we obtain

$$
U^T(\tau) = (X^T(\tau), V^T(\tau)) = \lim_{\epsilon \to 0} \sum_{n=-\infty}^{\infty} \langle \tilde{X}^T(\omega_n), \tilde{V}^T(\omega_n) \rangle e^{-i\omega_n \epsilon}.
$$

For large $\tau$ we note that $(1/\tau) \sum_n G^+(\omega_n) e^{-i\omega_n \epsilon} = 0$ which follows from converting the summation into an integral and noting that all the poles of $G^+(\omega_n)$ lie in the upper half-plane. Hence we get

$$
U^T(\tau) = (X^T(\tau), V^T(\tau)) = \sum_{n=-\infty}^{\infty} \langle [G^+\tilde{\eta}]^T, i\omega[G^+\tilde{\eta}]^T \rangle e^{-i\omega_n \epsilon}
$$

$$
= \sum_{n=-\infty}^{\infty} e^{-i\omega_n \epsilon} [F_2^T \tilde{\eta}_L + F_3^T \tilde{\eta}_R],
$$

(36)

where

$$
F_2^T = (G_{1,1}^+, G_{2,1}^+, \ldots, G_{N,1}^+, i\omega G_{1,1}^+, i\omega G_{2,1}^+, \ldots, i\omega G_{N,1}^+),
$$

(37)

$$
F_3^T = (G_{1,N}^+, G_{2,N}^+, \ldots, G_{N,N}^+, i\omega G_{1,N}^+, i\omega G_{2,N}^+, \ldots, i\omega G_{N,N}^+).
$$

(38)

Hence we get $E(\tau)$ in (35) as

$$
E(\tau) = -\lambda Q - i \sum_{n=-\infty}^{\infty} e^{-i\omega_n \epsilon} [\sigma^T F_2^T \tilde{\eta}_L + \sigma^T F_3^T \tilde{\eta}_R].
$$

(39)

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After using the full expression for $\tilde{v}_1(\omega)$ from (33) to evaluate $Q$ in (19), we obtain

$$E(\tau) = s_0 + \sum_{n=1}^{\infty} (s_n + s_{-n}) \quad \text{where} \quad (s_n + s_{-n}) \quad \text{has the following quadratic form:}
$$

$$s_n + s_{-n} = -\lambda \tau \xi_n^T A_n \xi_n + \xi_n^T \alpha_n + \alpha_n^T \xi_n + \frac{2\lambda \gamma_L}{\tau} |f_n|^2,
$$

where the matrix $A_n$ is given by (21) and

$$\alpha_n = \lambda \left( \begin{array}{c}
2i\gamma_L \omega G_{1,1}^+ - 1 \\
2i\gamma_L \omega G_{1,N}^+
\end{array} \right) F_1^T \Delta U - i e^{-i\omega T} \left( \begin{array}{c}
F_2^T \sigma \\
F_3^T \sigma
\end{array} \right),
$$

$$f_n = F_1^T \Delta U,
$$

where $F_1, F_2$ and $F_3$ are given by (34), (37) and (38) respectively.

Similarly, one can express $s_0$ as

$$s_0 = -\frac{\lambda \tau}{2} s_0^T A_0 s_0 + \alpha_0^T \xi_0 + \frac{\lambda \gamma_L}{\tau} f_0^2,
$$

where $A_0, \alpha_0, \xi_0$ and $f_0$ are all real.

We now first evaluate averages with respect to the Gaussian distribution given in (23) for $n \neq 0$ and with the distribution given in (29) for $n = 0$. We get

$$\langle e^{(s_n+s_{-n})} \rangle_{U,0} = \frac{1}{\det(I + \lambda \tau DA_n)} \exp \left[ \alpha_n^T (D^{-1} + \lambda \tau A_n)^{-1} \alpha_n + \frac{2\lambda \gamma_L}{\tau} |f_n|^2 \right] \quad \text{n} \neq 0,
$$

$$\langle e^{s_0} \rangle_{U,0} = \sqrt[12]{\det(I + \lambda \tau DA_0)} \exp \left[ \frac{1}{2} \alpha_0^T (D^{-1} + \lambda \tau A_0)^{-1} \alpha_0 + \frac{\lambda \gamma_L}{\tau} |f_0|^2 \right].
$$

Hence we get

$$\langle e^{E(\tau)} \rangle_{U,0} = \exp \left( -\frac{1}{2} \sum_{n=-\infty}^{\infty} \ln[\det(I + \lambda \tau DA_n)] \right)
\times \exp \left( \sum_{n=-\infty}^{\infty} \left[ \frac{1}{2} \alpha_n^T (D^{-1} + \lambda \tau A_n)^{-1} \alpha_n + \frac{\lambda \gamma_L}{\tau} |f_n|^2 \right] \right).
$$

After evaluating the required matrix inverse and determinant, we take the large $\tau$ limit to replace all the summations over $n$ by integrations over $\omega$. This yields

$$\langle e^{E} \rangle_{U,0} \sim e^{\mu(\lambda)} \exp \left( \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left[ \frac{dL_d dR}{1 + T_L T_R \lambda (\Delta \beta - \lambda) T(\omega)} + \lambda \gamma_L |f(\omega)|^2 \right] \right),
$$

where $\mu(\lambda)$ is given by (11) and

$$C(\omega) = \left( \begin{array}{cc}
\frac{1}{dL} - 4\lambda \gamma_L \omega^2 |G_{1,N}^+|^2 & 4\lambda \gamma_L \omega^2 G_{1,1}^+ G_{1,N}^+ + 2\lambda \omega G_{1,N}^-
\\
4\lambda \gamma_L \omega^2 G_{1,1}^+ G_{1,N}^- - 2\lambda \omega G_{1,N}^+ & \frac{1}{dR} + 4\lambda \gamma_R \omega^2 |G_{1,N}^+|^2
\end{array} \right).
$$

We see from (41) and (42) that $\alpha(\omega), f(\omega)$ are linear in $\Delta U$ and $\sigma$. After some algebraic manipulations and use of the identity (22) we then arrive at the following compact expression for $\langle e^{E} \rangle_{U,0}$:

$$\langle e^{E} \rangle_{U,0} \sim e^{\mu(\lambda)} \exp \left( -\frac{1}{2} \sigma^T H_1 \sigma + i \Delta U^T H_2 \sigma + \frac{1}{2} \Delta U^T H_3 \Delta U \right),
$$

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where

\[ H_1(\lambda) = \frac{1}{2} (I_1 + I_1^T), \]

with \( I_1(\lambda) = \frac{d_L d_R}{\pi} \int_{-\infty}^{\infty} d\omega \frac{C_{1,1} F_2 F_2^\dagger + C_{1,2} F_3 F_3^\dagger + C_{2,1} F_2 F_3^\dagger + C_{2,2} F_3 F_3^\dagger}{1 + T_L T_R \lambda (\Delta \beta - \lambda) T(\omega)}, \]

\[ H_2(\lambda) = \lim_{\epsilon \to 0} \frac{\lambda}{\pi} \int_{-\infty}^{\infty} d\omega \times e^{i\omega} \frac{d_l (1 - 2i\omega \gamma_L G_{1,1}^\dagger) F_1^* F_2^\dagger - 2i\omega (\gamma_L + \lambda d_l) d_R G_{1,n}^\dagger F_2 F_3^\dagger}{1 + T_L T_R \lambda (\Delta \beta - \lambda) T(\omega)}, \]

and

\[ H_3(\lambda) = \frac{1}{2} (I_3 + I_3^T), \]

with \( I_3(\lambda) = \frac{\lambda (\gamma_L + \lambda d_L)}{\pi} \int_{-\infty}^{\infty} d\omega \frac{F_1 F_1^\dagger}{1 + T_L T_R \lambda (\Delta \beta - \lambda) T(\omega)}. \]

Finally to get \( Z(\lambda, U, \tau | U_0) \) we substitute the expression for \( \langle e^Y \rangle_{U,U_0} \) from (47) into (35) and perform the Gaussian integration over \( \sigma \). This gives

\[ Z(\lambda, U, \tau | U_0) \sim \frac{e^{\tau \mu(\lambda)}}{(2\pi)^N \sqrt{\det H_1}} e^{(1/2)U^T H_6 U} e^{-(1/2)(U^T + \Delta U^T) H_1^{-1}(U + H_2^T \Delta U)}. \]

Putting \( \lambda = 0 \) in the above expression gives the steady state distribution as

\[ P_{SS}(U) = Z(0, U, \tau \to \infty | U_0) = \frac{\exp(-U^T H_1^{-1}(0) U)}{(2\pi)^N \sqrt{\det H_1(0)}}. \]

From the long time solution in (36) it can be directly verified that

\[ \lim_{t \to -\infty} \langle UU^T \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega [d_L F_2 F_2^\dagger + d_R F_3 F_3^\dagger], \]

and using the fact that \( \langle UU^T \rangle \) is real we see that the above equals \( H_1(0) \), consistently with (52).

Now, according (8), the initial and the final variables \( U_0 \) and \( U \) in (51) must factorize, which implies \([H_3 - H_2 H_1^{-1} H_2^T - H_1^{-1} H_1^T] + [H_3 - H_2 H_1^{-1} H_2^T - H_2 H_1^{-1}] = 0\). Since \( H_1 \) and \( H_3 \) are symmetric matrices, the above condition can be expressed as

\[ H_3 - H_2 H_1^{-1} H_2^T - H_1^{-1} H_1^T = 0. \]

Using this (51) gives

\[ Z(\lambda, U, \tau | U_0) \sim \frac{e^{\tau \mu(\lambda)}}{(2\pi)^N \sqrt{\det H_1(\lambda)}} \exp \left( -\frac{1}{2} U^T L_1(\lambda) U \right) \exp \left( -\frac{1}{2} U_0^T L_2(\lambda) U_0 \right). \]

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This means that we can make the following identifications for $\Psi(U, \lambda), \chi(U_0, \lambda)$:

$$\Psi(U, \lambda) = \frac{1}{(2\pi)^N \sqrt{\det H_1(\lambda)}} \exp \left( -\frac{1}{2} U^T L_1(\lambda) U \right),$$  \hspace{1cm} (55)

$$\chi(U_0, \lambda) = \exp \left( -\frac{1}{2} U_0^T L_2(\lambda) U_0 \right),$$  \hspace{1cm} (56)

where $L_1(\lambda) = H_1^{-1} + H_1^{-1} H_2^T$ and $L_2(\lambda) = H_2 H_1^{-1} H_2^T - H_3 = -H_1^{-1} H_2^T$.  \hspace{1cm} (57)\hspace{1cm} (58)

Thus we have obtained the left and right eigenvectors of the Fokker–Planck operator $L_\lambda$ corresponding to the eigenvalue $\mu(\lambda)$. It can be seen that the orthonormality condition $\int dU \chi(U, \lambda) \Psi(U, \lambda) = 1$ is satisfied.

We obtain $Z(\lambda)$ by integrating $Z(\lambda, U, \tau|U_0)$ over $U$ and then averaging over the initial condition $U_0$ with respect to the steady state distribution $P_{SS}(U_0)$. This then gives our final expression for the correction to the CGF:

$$g(\lambda) = (\det H_1(\lambda) \det H_1(0) \det L_1(\lambda) \det [H_1^{-1}(0) + L_2(\lambda)])^{-1/2}. \hspace{1cm} (59)$$

Since $L_1(0) = H_1^{-1}(0)$ and $L_2(0) = 0$, it is verified that $g(0) = 1$.

5. The example of a single Brownian particle

The Langevin equation for a single Brownian particle is given by

$$m\ddot{v} = -(\gamma_L + \gamma_R)v + \eta_L(t) + \eta_R(t), \hspace{1cm} (60)$$

where $v$ is the velocity of the particle and $m$ is its mass. Here we consider the velocity of the particle not the position, since the velocity $v$ of the particle will have a normalized steady state distribution whereas the position will not have and the heat transfer $Q$, in which we are interested, does not depend on the position. For a single Brownian particle the matrix defined in (13) becomes a complex number: $G^+(\omega) = 1/(-m\omega^2 + i\omega\gamma)$ where $\gamma = \gamma_L + \gamma_R$. Following all the steps described in section 6 one can easily arrive at the expression (47), where $\mu(\lambda)$ is given in (11) and the $H_s$ are given in (48)–(50). In this case one can carry out the integrations present in the expressions of all these quantities. The expression for phonon transmission coefficient is obtained from (12) and given by $T(\omega) = 4\gamma_L\gamma_R[m^2\omega^2 + (\gamma_L + \gamma_R)^2]^{-1}$. We use this form in (11) to evaluate the integral and get

$$\mu(\lambda) = \frac{\gamma_L + \gamma_R}{2m} \left[ 1 - \sqrt{1 + \frac{4\gamma_L\gamma_R}{(\gamma_L + \gamma_R)^2} T_L T_R \lambda (\Delta\beta - \lambda)} \right].$$  \hspace{1cm} (61)

This is the result obtained in [16]. Similarly using $G^+(\omega) = 1/(-m\omega^2 + i\omega\gamma)$ and the above form for $T(\omega)$ we evaluate $H_s$ given by (48)–(50) to get

$$H_1 = \frac{d_L + d_R}{m\sqrt{\gamma^2 + a^2}}, \hspace{1cm} H_2 = \frac{\lambda d_L + (1/2)(\gamma - \sqrt{\gamma^2 + a^2})}{\sqrt{\gamma^2 + a^2}},$$

$$H_3 = \frac{m\lambda}{\sqrt{\gamma^2 + a^2}}(\gamma_L + \lambda d_L), \hspace{1cm} \text{where, } a = \sqrt{4d_L d_R \lambda (\Delta\beta - \lambda)}. \hspace{1cm} (62)$$
It is easily verified that the $H$s for the single Brownian particle satisfy the relation (53), i.e. $(H_2)^2 + H_2 - H_1 H_3 = 0$. Now using the expression (59) we obtain

$$g(\lambda) = 2 \sqrt{\frac{\gamma \sqrt{\gamma^2 + 4 d_L d_R \lambda (\Delta \beta - \lambda)}}{(\gamma + \sqrt{\gamma^2 + 4 d_L d_R \lambda (\Delta \beta - \lambda)})^2 - 4 \lambda^2 d_L^2}}, \quad (63)$$

which also agrees with the result in [16].

6. Discussion

We have presented a formalism for calculating the CGF $\mu(\lambda)$ and its correction $g(\lambda)$ for heat transport across a harmonic chain connected to white-noise Langevin reservoirs. The formula for $\mu(\lambda)$ is expressed as an integral over frequencies, with the integrand depending explicitly on the phonon transmission function $T(\omega)$. The expression for $g(\lambda)$ is in terms of integrals involving an appropriate phonon Green’s function. We have illustrated the usefulness of the formalism by calculating $\mu(\lambda)$ and $g(\lambda)$ for a single Brownian particle for which case all integrals can be performed explicitly. For systems with a greater number of particles, the function $T(\omega)$ can easily be obtained analytically for an ordered harmonic chain and numerically for disordered harmonic chains. Hence our formalism can be used to numerically compute $\mu(\lambda)$ and $g(\lambda)$ with high accuracy. A knowledge of these functions would enable one to check the validity of the fluctuation symmetry for the large deviation function. We note that $\mu(\lambda)$ itself is a useful quantity, containing information on current moments in the nonequilibrium state. We show that it always satisfies the fluctuation symmetry relation. Finally we have pointed out that $\mu(\lambda)$ can, in general, be shown to be the largest eigenvalue of a Fokker–Planck type operator ($L_\lambda$ for our problem). Using our formalism we obtain not only this eigenvalue but also the corresponding left and right eigenvectors.

The present approach has recently been generalized to the problem of computing $\mu(\lambda)$ for the case of heat conduction across arbitrary harmonic networks [40]. The problem of calculating $g(\lambda)$ in such cases and also the extension of the present formalism to quantum systems are interesting open problems.

Appendix A. The Fokker–Planck equation

Let $P(Q, U, t|U_0)$ denote the probability distribution of heat flow $Q$ in duration $\tau$ given the initial and final configurations $U$ and $U_0$ respectively. The distribution $P(Q, U, t|U_0)$ satisfies the following Fokker–Planck equation:

$$\frac{\partial P}{\partial t} = \left[ -\sum_{i=1}^{2N} \frac{\partial}{\partial U_i} \frac{\langle \Delta U_i \rangle}{\Delta t} - \frac{\partial}{\partial Q} \frac{\langle \Delta Q \rangle}{\Delta t} + \frac{1}{2} \sum_{i=1}^{2N} \sum_{m=1}^{2N} \frac{\partial^2}{\partial U_i \partial U_m} \frac{\langle \Delta U_i \Delta U_m \rangle}{\Delta t} \right. \left. + \sum_{i=1}^{2N} \frac{\partial^2}{\partial U_i \partial Q} \frac{\langle \Delta U_i \Delta Q \rangle}{\Delta t} + \frac{\partial^2}{\partial Q^2} \frac{\langle \Delta Q^2 \rangle}{\Delta t} \right] P(Q, U, t|U_0); \quad \text{with } \Delta t \to 0,$$

(A.1)
where the moments are calculated using the Langevin equations (4) and heat equation given in (6). After calculating the moments we get
\[
\frac{\partial P}{\partial t} = \mathcal{L}_Q P(Q, U, t|U_0)
\]
where
\[
\mathcal{L}_Q = \sum_{l=1}^{N} \frac{1}{m_l} \left[ \frac{\partial H}{\partial x_l} \frac{\partial \rho}{\partial v_l} - \frac{\partial H}{\partial v_l} \frac{\partial \rho}{\partial x_l} \right] + \gamma_l \frac{\partial}{\partial v_1} v_1 + \frac{\gamma_R}{m_N} \frac{\partial}{\partial v_N} v_N + \left( \frac{\gamma_L v_1}{m_1} - \frac{\gamma_L T_l}{m_1} \right) \frac{\partial}{\partial Q} + \frac{\gamma_L T_l}{m_1} \frac{\partial^2}{\partial v_1^2} + \frac{\gamma_R T_R}{m_2} \frac{\partial^2}{\partial v_2^2} + \frac{\gamma_L T_l}{m_1} \frac{\partial^2}{\partial Q^2} + 2 \frac{\gamma_L T_l}{m_1} \frac{\partial^2}{\partial v_1 \partial Q} v_1.
\]
The corresponding Fokker–Planck equation for the restricted characteristic function $Z(\lambda, U, \tau|U_0) = \int_{-\infty}^{\infty} dQ e^{-\lambda Q} P(Q, U, t|U_0)$ is obtained by multiplying both sides of the above equation by $e^{-\lambda Q}$ and then integrating with respect to $Q$. We get
\[
\frac{\partial}{\partial \tau} Z(\lambda, U, \tau|U_0) = \mathcal{L}_\lambda Z(\lambda, U, \tau|U_0)
\]
where
\[
\mathcal{L}_\lambda = \sum_{l=1}^{N} \frac{1}{m_l} \left[ \frac{\partial H}{\partial x_l} \frac{\partial \rho}{\partial v_l} - \frac{\partial H}{\partial v_l} \frac{\partial \rho}{\partial x_l} \right] + \gamma_l \frac{\partial}{\partial v_1} v_1 + \frac{\gamma_R}{m_N} \frac{\partial}{\partial v_N} v_N + \left( \frac{\gamma_L v_1}{m_1} - \frac{d_l}{m_1} \right) \lambda + \frac{d_l}{m_1} \frac{\partial^2}{\partial v_1^2} + \frac{d_R}{m_2} \frac{\partial^2}{\partial v_2^2} + \frac{d_L v_1^2}{m_1} + \frac{2 d_l}{m_1} \frac{\partial}{\partial v_1} v_1.
\]

Appendix B. The multi-dimensional Gaussian integral of complex variables

For ease of reference we give the following result for complex Gaussian integrals:
\[
\int d^n Z \exp(-Z^T A Z^* + Z^T B + C^T Z^*) = \frac{\pi^n}{\det A} \exp(C^T A^{-1} B)
\]
where $Z$ is an $n$-dimensional complex vector, $A$ is a Hermitian matrix and $B, C$ are arbitrary complex $n$-dimensional vectors. The integration $\int d^n Z$ denotes the real integrations $\int d^n X d^n Y$ with the substitution $Z = X + iY$, $X$ and $Y$ being real $n$-dimensional vectors.

**Proof.** Let $K$ be the unitary matrix such that $A = K D K^\dagger$ where $D$ is a diagonal matrix with all real diagonal elements. Now with the following transformations:
\[
\tilde{Z} = K^T Z, \quad \tilde{B} = K^T B, \quad \tilde{C} = K^T C
\]
we can write the complex Gaussian integration in the form
\[
\int_{-\infty}^{\infty} d^n \tilde{X} d^n \tilde{Y} \exp(-\tilde{Z}^T D \tilde{Z}^* + \tilde{Z}^T \tilde{B} + \tilde{C}^T \tilde{Z}^*).
\]
Since $D$ is diagonal, the above is a product of $2n$ uncoupled Gaussian integrations. Performing the integrations we get
\[
\prod_{i=1}^{n} \pi \frac{\det B_i C_i}{D_i} = \frac{\pi^n}{\det A} \exp(C^T D^{-1} B) = \frac{\pi^n}{\det A} \exp(C^T A^{-1} B),
\]
which completes the proof. \qed
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