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Thermal averages of expressions involving exponentials of quadratic and linear boson operators

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Abstract. We present a new technique to calculate ensemble averages of exponentials of quadratic boson operators, possibly multiplied by exponentials of linear boson operators. The method is based on the use of coherent states in the evaluation of matrix elements. Although this is a very simple basic idea, the technique enables the exact evaluation of several complicated averages from the theory of exciton transport. These averages, which could previously be given only approximately, are treated as examples to discuss the features of the method.

1. Introduction

The necessity to calculate thermal averages of exponential operators arises in theories describing systems whose coupling to a bath is partially taken into account through a unitary transformation of the Hamiltonian and the wavefunctions [1-7]. Since a description of the system alone is derived, an appropriate average over the bath has to be chosen as the Hamiltonian of the unperturbed system. The small-polaron theory [8] is one example of the successful application of this concept.

In the simple theories a thermal average of an exponential of linear phonon operators has to be taken. This average can be found in the standard references [9]. In more advanced theories [10] the unitary transformation employed contains exponentials of quadratic phonon operators in addition to the usual linear phonon operators characteristic of the small-polaron case.

For exponential quadratic operators, not many averaging methods are available [11]. Of the three techniques given in [11], none is particularly well suited for the calculation of averages containing exponentials of quadratic *and* of linear phonon operators. In fact, the most versatile of the methods from [11], the matrix technique, is not applicable at all in this case. The coordinate-momentum representation technique leads to complicated exponentials of differential operators which are not readily evaluated in each case. Finally, the so-called operator disentangling technique, which we prefer to call the occupation number representation method, because our method also involves operator disentangling, often yields many sums over intermediate states, making the recognition of compact underlying structures virtually impossible. The method that we describe in this paper avoids these disadvantages and still gives results where the other techniques fail.

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2. The technique

Our technique is a combination of operator disentangling, occupation number representation and, a new feature, the coherent state representation. In order to demonstrate it, we will calculate a simple example. Consider the unitary transformation

$$U_q = \theta_q \psi_q \tag{1}$$

$$\theta_q = \exp[2G_q(b_q b_{-q} - b_q^+ b_{-q}^+)] \qquad G_q = G_q^* \tag{2}$$

$$\psi_q = \exp[-c_q(b_q - b_{-q}^+) - c_{-q}(b_{-q} - b_q^+)] \qquad c_{-q} = c_q^*. \tag{3}$$

This transformation occurs as a factor of the total unitary transformation in theories in which the latter couples only phonons of opposite wavevectors. We assume a canonical ensemble (or a grand canonical one with vanishing chemical potential)

$$\rho = \frac{1}{Z}\exp\left(-\sum_q \beta\hbar\omega_q b_q^+ b_q\right) \qquad \omega_q = \omega_{-q} \tag{4}$$

where Z is the usual partition function.

First, we wish to case U_q in an ordered form. Whereas normal or antinormal ordering is not difficult for exponentials of *linear* phonon operators such as ψ_q, it may become very tedious, if not unfeasible, for exponentials of quadratic phonon operators. A general method for *canonical decomposition* of these transformations, involving the exponentiation and inversion of potentially large matrices, has been given by Balian and Brézin [12]. Canonical decomposition means factorisation in a pure creation, a diagonal and a pure destruction part, corresponding to partial (and enabling full) normal ordering. Applying their result (equations (39)-(42) of [12]) to the homogeneous transformation θ_q, we have to deal with 4×4 matrices only and obtain

$$\langle\theta_q\psi_q\rangle = \frac{1}{Z_{q,-q}}\frac{\exp(|c_q|^2)}{\cosh 2G_q} T \tag{5a}$$

$$\begin{aligned} T \equiv \mathrm{Tr}_{q,-q}\{&\exp[-d(b_q^+ b_q + b_{-q}^+ b_{-q})]\exp(e_1 b_q b_{-q})\exp(f_1 b_q)\exp(g_1 b_{-q}) \\ &\times \exp(e_2 b_q^+ b_{-q}^+)\exp(f_2 b_q^+)\exp(g_2 b_{-q}^+)\} \end{aligned} \tag{5b}$$

with

$$\begin{aligned} d &= \beta\hbar\omega_q + \ln\cosh 2G_q \qquad & e_1 &= \tanh 2G_q \\ e_2 &= -\exp(-2\beta\hbar\omega_q)\tanh 2G_q \qquad & f_1 &= -f_2^* = g_1^* = -g_2 = -c_q. \end{aligned} \tag{5c}$$

In (5*b*) we have shifted operators using the cyclic property of the trace which is now only over the $+q$ and $-q$ states. $Z_{q,-q}$ is the partition function corresponding to these two wavevectors: $Z_{q,-q} = 1/[1-\exp(-\beta\hbar\omega_q)]^2$. We will concentrate on the quantity T. The trace is written with occupation number states and a pair of complete sets of coherent states [13]

$$\int \frac{d^2\alpha}{\pi}|\alpha\rangle\langle\alpha| = 1 \tag{6}$$

is inserted between the destruction and creation operators:

$$\begin{aligned} T = \sum_{n_q, n_{-q}} \iint &\frac{d^2\alpha_q}{\pi}\frac{d^2\alpha_{-q}}{\pi}\langle n_q, n_{-q}|\exp[-d(n_q + n_{-q})] \\ &\times \exp(e_1\alpha_q\alpha_{-q})\exp(f_1\alpha_q)\exp(g_1\alpha_{-q})|\alpha_q, \alpha_{-q}\rangle \\ &\times \langle\alpha_q, \alpha_{-q}|\exp(e_2\alpha_q^*\alpha_{-q}^*)\exp(f_2\alpha_q^*)\exp(g_2\alpha_{-q}^*)|n_q, n_{-q}\rangle. \end{aligned} \tag{7}$$

In (7) we have made use of the fact that coherent states are the eigenstates of the destruction operators [13]:

$$b|\alpha\rangle = \alpha|\alpha\rangle. \tag{8}$$

The overlaps of the occupation number and coherent states are simple expressions [13]

$$\langle n|\alpha\rangle = \exp(-\tfrac{1}{2}|\alpha|^2)\frac{\alpha^n}{\sqrt{n!}} \tag{9}$$

which enable the immediate evaluation of the sums over occupation numbers

$$\sum_n \mathrm{e}^{-dn}|\langle n|\alpha\rangle|^2 = \exp[(\mathrm{e}^{-d}-1)|\alpha|^2]. \tag{10}$$

Renaming α_q to α_1, α_{-q} to α_2, we obtain

$$T = \frac{1}{\pi^2}\int \mathrm{d}^2\alpha_1 \int \mathrm{d}^2\alpha_2 \exp(e_2\alpha_1^*\alpha_2^*)\exp[(\mathrm{e}^{-d}-1)(\alpha_1^*\alpha_1+\alpha_2^*\alpha_2)]\exp(e_1\alpha_1\alpha_2)$$
$$\times\exp(f_2\alpha_1^*)\exp(f_1\alpha_1)\exp(g_2\alpha_2^*)\exp(g_1\alpha_2). \tag{11}$$

Decomposition of the α into their real and imaginary parts

$$\alpha_k = x_k + \mathrm{i}y_k \qquad k = 1, 2 \tag{12}$$

obviously transforms the integral in a multiple Gaussian integral of the general form

$$I = \int \mathrm{d}^{2N}x \exp(-\boldsymbol{x}^{\mathrm{T}}\mathbf{A}\boldsymbol{x} + \boldsymbol{x}^{\mathrm{T}}\boldsymbol{v}) \tag{13}$$

where $\boldsymbol{x}^{\mathrm{T}} = (x_1, y_1, x_2, y_2)$, $N = 2$ and $\mathbf{A}$ and $\boldsymbol{v}$ are a matrix and a column vector determined by the coefficients d, e_1, e_2, etc. A superscript T denotes the transpose of a matrix or vector.

Without restriction of generality, $\mathbf{A}$ can be chosen symmetric. Then the integral can be evaluated (under conditions ensuring its convergence):

$$I = \pi^N \frac{1}{(\det\mathbf{A})^{1/2}}\exp(\tfrac{1}{4}\boldsymbol{v}^{\mathrm{T}}\mathbf{A}^{-1}\boldsymbol{v}). \tag{14}$$

Of course, we do not want to perform the transformation from the variables α to x explicitly in each case we are encountering. Therefore, we derive a formula directly applicable to (11). This can be simply done by using the connection of $\boldsymbol{x}$ and $\boldsymbol{\alpha}$ through a unitary transformation:

$$\begin{pmatrix} x_k \\ y_k \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ -\mathrm{i} & \mathrm{i} \end{pmatrix}\begin{pmatrix} \alpha_k \\ \alpha_k^* \end{pmatrix} \equiv \frac{1}{\sqrt{2}}\mathbf{U}_k\begin{pmatrix} \alpha_k \\ \alpha_k^* \end{pmatrix}. \tag{15}$$

From (15), we have

$$\boldsymbol{x} = \frac{1}{\sqrt{2}}\mathbf{U}\boldsymbol{\alpha} \tag{16}$$

where $\mathbf{U}$ is the $2N\times 2N$ matrix having N 2×2 blocks $\mathbf{U}_k$ on its diagonal and zero elements elsewhere.

Using this relation we obtain

$$\boldsymbol{x}^{\mathrm{T}}\mathbf{A}\boldsymbol{x} = \boldsymbol{\alpha}^{+}\mathbf{B}\boldsymbol{\alpha} \tag{17a}$$

with

$$\mathbf{B} = \tfrac{1}{2}\mathbf{U}^{+}\mathbf{A}\mathbf{U} \tag{17b}$$

where $\boldsymbol{\alpha}^{+} = (\alpha_1^*, \alpha_1, \alpha_2^*, \alpha_2)$, and a superscript +, of course, means the Hermitian conjugate of a matrix or vector. From (17*b*) it is evident that

$$\det \mathbf{A} = \det 2\mathbf{B} \tag{18}$$

because $\mathbf{U}$ is unitary. The matrix $\mathbf{B}$ can now be obtained directly from (11). However, this expression does not determine $\mathbf{B}$ uniquely, since in the form $\boldsymbol{\alpha}^{+}\mathbf{B}\boldsymbol{\alpha}$ elements like $\alpha_k^*\alpha_l^*(k \neq l)$ or $\alpha_k^*\alpha_l$ (k, l arbitrary) appear twice. This ambiguity is resolved by recognising that the symmetry of $\mathbf{A}$ implies the condition

$$(\boldsymbol{\sigma}\mathbf{B})^{\mathrm{T}} = \boldsymbol{\sigma}\mathbf{B} \tag{19a}$$

where $\boldsymbol{\sigma}$ is the $2N \times 2N$ matrix having the blocks

$$\boldsymbol{\sigma}_k = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{19b}$$

on its diagonal. This condition means that the matrix $\boldsymbol{\sigma}\mathbf{B}$, obtained from $\mathbf{B}$ by interchanging the odd with the even rows, has to be symmetric. Because of

$$\boldsymbol{x}^{\mathrm{T}}\boldsymbol{v} = \boldsymbol{x}^{+}\boldsymbol{v} = (1/\sqrt{2})\boldsymbol{\alpha}^{+}\mathbf{U}^{+}\boldsymbol{v} \equiv \boldsymbol{\alpha}^{+}\boldsymbol{z} \tag{20}$$

we can write the whole integral in terms of $\mathbf{B}$:

$$I = \pi^{N}\frac{1}{(\det 2\mathbf{B})^{1/2}}\exp(\tfrac{1}{4}\boldsymbol{z}^{\mathrm{T}}\boldsymbol{\sigma}\mathbf{B}^{-1}\boldsymbol{z}). \tag{21}$$

(Note that $\mathbf{U} = \mathbf{U}^*\boldsymbol{\sigma}$.) The vector $\boldsymbol{z}$ is uniquely determined from (11). Formula (21), however, is not yet simple enough. Since we do not want to calculate the full inverse of $\mathbf{B}$ just to get the quadratic form in the exponent, we use the identity

$$\boldsymbol{u}^{\mathrm{T}}\mathbf{M}^{-1}\boldsymbol{w} = -\frac{1}{\det \mathbf{M}}\det\begin{pmatrix} 0 & \boldsymbol{u}^{\mathrm{T}} \\ \boldsymbol{w} & \mathbf{M} \end{pmatrix} \tag{22}$$

where the second matrix on the right-hand side is obtained from $\mathbf{M}$ by adding one row and one column in the indicated way. Equation (22) is easily proved by expanding the numerator determinant with respect to the added row and column and using the well known explicit expression for the inverse of a matrix. Employing (22), we can cast our result in the form

$$T = \frac{1}{(\det 2\mathbf{B})^{1/2}}\exp\left(-\frac{1}{2}\frac{\det 2\mathbf{D}}{\det 2\mathbf{B}}\right) \tag{23a}$$

where

$$\mathbf{D} = \begin{pmatrix} 0 & \tfrac{1}{2}\boldsymbol{z}^{\mathrm{T}}\boldsymbol{\sigma} \\ \tfrac{1}{2}\boldsymbol{z} & \mathbf{B} \end{pmatrix}. \tag{23b}$$

In our case, $\mathbf{D}$ is the following 5×5 matrix:

$$\mathbf{D} = \frac{1}{2}\begin{bmatrix} 0 & f_1 & f_2 & g_1 & g_2 \\ f_2 & 1-e^{-d} & 0 & 0 & -e_2 \\ f_1 & 0 & 1-e^{-d} & -e_1 & 0 \\ g_2 & 0 & -e_2 & 1-e^{-d} & 0 \\ g_1 & -e_1 & 0 & 0 & 1-e^{-d} \end{bmatrix} \tag{24}$$

where the 4×4 matrix obtained by crossing out the first row and column is $2\mathbf{B}$, of course.

The expressions in (23) are now easily evaluated, giving the final result

$$T = \frac{1}{(1-e^{-d})^2 - e_1 e_2} \times \exp\left(\frac{1}{(1-e^{-d})^2 - e_1 e_2}[(1-e^{-d})(f_1 f_2 + g_1 g_2) + e_2 f_1 g_1 + e_1 f_2 g_2]\right). \qquad (25)$$

We can therefore summarise the method as follows. The first step consists in operator disentangling, aiming at an expression containing one *antinormally* ordered group of operators and diagonal operators outside this group (see (5*b*)). The second step is using occupation number states for the evaluation of the trace to convert the diagonal operators into numbers and inserting coherent states between the destruction and creation operators. The occupation number sums can always be performed for exponential operators and we are left with an integral expression that can always be transformed to a multiple Gaussian integral. In a third step the integral is reduced to a determinant expression. Often the reduction of these determinants to simple formulae will be the biggest problem of the calculation.

As a first step we can equivalently arrange the operators in *normal* ordering and sandwich the diagonal operator between the creation or destruction operators. In this case, the second step will be to express the trace as an integral over coherent states and to insert a complete set of occupation number states next to the diagonal operator. In our simple case, one kind of expression can be obtained from the other through a simple application of the cyclic property of the trace. We will, however, look at a more complicated case later where one direction of ordering is to be preferred over the other.

In calling our example simple, we are aware of the fact that by the transformation

$$b_+ = \frac{1}{\sqrt{2}}(b_q + b_{-q}) \qquad b_- = \frac{1}{\sqrt{2}}(b_q - b_{-q}) \qquad (26)$$

the trace in (5) can be broken down in two factor traces over single phonon branches. Each of these traces corresponds to an even simpler case than the one considered, since $\mathbf{B}$ and $\mathbf{D}$ are 2×2 and 3×3 matrices, respectively. However, the symmetry properties of $\mathbf{B}$ are more clearly visible in the slightly more complicated form and the calculational effort for the evaluation of the full problem (5) is less than for the factorisation plus evaluation of two factor traces. It may be noted that even these simple factor traces are not straightforwardly evaluated within either the occupation number or the coordinate-momentum representation techniques. With the latter, the calculation is feasible due to the special form of the operator θ_q (2). To evaluate the factor traces of (5*b*) with *general* coefficients, *d, e, f, g*, however, seems a very difficult objective within this method, involving the evaluation of rather complicated differential operators.

The occupation number technique leads to five nested sums, of which only two can be evaluated immediately. The remaining sums look tangled. Even verifying that they represent the simple analytical result, known through the other techniques, is an intricate matter. Obtaining the analytical formula from these sums in the first place seems to be beyond hope.

3. Examples

We now apply our technique to the calculation of several averages of interest in the theory of exciton transport with quadratic phonon coupling [10]. First, we wish to consider the quantity $\langle\theta_n^+\theta_m\rangle$, for $n \neq m$, where

$$\theta_n = \exp[-\gamma(b_n^2 - b_n^{+2})]. \tag{27}$$

What makes the calculation of this average difficult and has until now prevented us doing it exactly (except for the dimer case) is that θ_n and θ_m are operators in site representation, whereas the density matrix is diagonal in momentum representation:

$$\rho = \frac{1}{Z}\exp\left(-\sum_\lambda \beta\hbar\omega_\lambda b_\lambda^+ b_\lambda\right). \tag{28}$$

The relations connecting the two representations are

$$b_n = \frac{1}{\sqrt{N}}\sum_\lambda \exp(-\mathrm{i}\lambda n) b_\lambda \qquad b_n^+ = \frac{1}{\sqrt{N}}\sum_\lambda \exp(\mathrm{i}\lambda n) b_\lambda^+ \tag{29}$$

and the corresponding inversion formulae (N is the number of phonon modes, n is a lattice vector, λ a wavevector). We proceed with the first step of our method, operator disentangling:

$$\theta_n^+\theta_m = \cosh 2\gamma \exp[\tfrac{1}{2}\tanh 2\gamma(b_n^2 - b_m^2)] \exp[\ln\cosh 2\gamma(b_n^+b_n + b_m^+b_m)] \times \exp[-\tfrac{1}{2}\tanh 2\gamma(b_n^{+2} - b_m^{+2})]. \tag{30}$$

This is antinormally ordered except for the diagonal middle part. In contrast to our simple introductory example, it is not useful now to commute the diagonal part past one of the enclosing operators to join it with the density operator, since the latter is diagonal in a different representation. However, we can achieve full antinormal ordering using the formula [13]

$$\exp(-ab^+b) = \mathrm{e}^a \sum_n \frac{1}{n!}(1-\mathrm{e}^a)^n b^n b^{+n}. \tag{31}$$

Transforming to momentum representation and proceeding to step two, we obtain

$$\begin{aligned}
\langle\theta_n^+\theta_m\rangle = \frac{1}{Z}\frac{1}{\cosh 2\gamma}\int\frac{\mathrm{d}^2\alpha_{\lambda_1}}{\pi}\cdots\int\frac{\mathrm{d}^2\alpha_{\lambda_N}}{\pi}
&\times\sum_{\{n_\lambda\}}\left\langle\{n_\lambda\}\right|\exp\left(\frac{1}{2N}t_\gamma\sum_{\lambda,\lambda'}\{\exp[-\mathrm{i}(\lambda+\lambda')n]-\exp[-\mathrm{i}(\lambda+\lambda')m]\}\alpha_\lambda\alpha_{\lambda'}\right)\\
&\times\sum_{l,j}\frac{d_\gamma^l}{l!}\frac{d_\gamma^j}{j!}\left(\frac{1}{\sqrt{N}}\sum_{\lambda'}\exp(-\mathrm{i}\lambda' n)\alpha_{\lambda'}\right)^l\left(\frac{1}{\sqrt{N}}\sum_{\lambda'}\exp(-\mathrm{i}\lambda' m)\alpha_{\lambda'}\right)^j\left|\{\alpha_\lambda\}\right\rangle\\
&\times\left\langle\{\alpha_\lambda\}\right|\left(\frac{1}{\sqrt{N}}\sum_\lambda\exp(\mathrm{i}\lambda n)\alpha_\lambda^*\right)^l\left(\frac{1}{\sqrt{N}}\sum_\lambda\exp(\mathrm{i}\lambda m)\alpha_\lambda^*\right)^j\\
&\times\exp\left(-\frac{1}{2N}t_\gamma\sum_{\lambda\lambda'}\{\exp[\mathrm{i}(\lambda+\lambda')n]-\exp[\mathrm{i}(\lambda+\lambda')m]\}\alpha_\lambda^*\alpha_{\lambda'}^*\right)\\
&\times\exp\left(-\sum_\lambda\beta\hbar\omega_\lambda n_\lambda\right)\left|\{n_\lambda\}\right\rangle
\end{aligned} \tag{32a}$$

where

$$d_\gamma = 1 - 1/\cosh 2\gamma \qquad t_\gamma = \tanh 2\gamma \tag{32b}$$

and $|\{n_\lambda\}\rangle$ and $|\{\alpha_\lambda\}\rangle$ indicate the product states over all N single phonon occupation number and coherent states, respectively.

As in the simple example the sums over occupation numbers can be done immediately, resulting in

$$\begin{aligned}\langle\theta_n^+\theta_m\rangle = \frac{1}{Z}\frac{1}{\cosh 2\gamma}\frac{1}{\pi^N}\int \mathrm{d}^2\alpha_{\lambda_1}\ldots\int \mathrm{d}^2\alpha_{\lambda_N}\\ \times\exp\left(-\frac{1}{2N}t_\gamma\sum_{\lambda\lambda'}\{\exp[\mathrm{i}(\lambda+\lambda')n]-\exp[\mathrm{i}(\lambda+\lambda')m]\}\alpha_\lambda^*\alpha_{\lambda'}^*\right)\\ \times\exp\left[\sum_{\lambda\lambda'}\left(-e_\lambda\delta_{\lambda\lambda'}+\frac{d_\gamma}{N}\{\exp[\mathrm{i}(\lambda-\lambda')n]+\exp[\mathrm{i}(\lambda-\lambda')m]\}\right)\alpha_\lambda^*\alpha_{\lambda'}\right]\\ \times\exp\left(\frac{1}{2N}t_\gamma\sum_{\lambda\lambda'}\{\exp[-\mathrm{i}(\lambda+\lambda')n]-\exp[-\mathrm{i}(\lambda+\lambda')m]\}\alpha_\lambda\alpha_{\lambda'}\right)\end{aligned} \tag{33a}$$

with

$$e_\lambda = 1-\exp(-\beta\hbar\omega_\lambda) = \frac{1}{n_\lambda+1} \tag{33b}$$

n_λ now being the thermal occupation number of mode λ.

From this expression we can immediately deduce the matrix $\mathbf{B}$ which can be written

$$\mathbf{B} = \begin{bmatrix}\mathbf{B}_{\lambda_1\lambda_1} & \mathbf{B}_{\lambda_1\lambda_2} & \cdots & \mathbf{B}_{\lambda_1\lambda_N}\\ \mathbf{B}_{\lambda_2\lambda_1} & \mathbf{B}_{\lambda_2\lambda_2} & \cdots & \mathbf{B}_{\lambda_2\lambda_N}\\ \vdots & \vdots & & \vdots\\ \mathbf{B}_{\lambda_N\lambda_1} & \mathbf{B}_{\lambda_N\lambda_2} & \cdots & \mathbf{B}_{\lambda_N\lambda_N}\end{bmatrix} \tag{34a}$$

where the $\mathbf{B}_{\lambda\lambda'}$ are the 2×2 matrices given by

$$\mathbf{B}_{\lambda\lambda'} = \frac{1}{2}\begin{bmatrix} e_\lambda\delta_{\lambda\lambda'}-\frac{d_\gamma}{N}\{\exp[\mathrm{i}(\lambda-\lambda')n]+\exp[\mathrm{i}(\lambda-\lambda')m]\} & \frac{1}{N}t_\gamma\{\exp[\mathrm{i}(\lambda+\lambda')n]-\exp[\mathrm{i}(\lambda+\lambda')m]\}\\ -\frac{1}{N}t_\gamma\{\exp[-\mathrm{i}(\lambda+\lambda')n]-\exp[-\mathrm{i}(\lambda+\lambda')m]\} & e_\lambda\delta_{\lambda\lambda'}-\frac{d_\gamma}{N}\{\exp[-\mathrm{i}(\lambda-\lambda')n]+\exp[-\mathrm{i}(\lambda-\lambda')m]\}\end{bmatrix}. \tag{34b}$$

Our result is, of course,

$$\langle\theta_n^+\theta_m\rangle = \frac{1}{Z}\frac{1}{\cosh 2\gamma}\frac{1}{\det 2\mathbf{B}} \tag{35}$$

so that we are left with the problem of evaluating the $2N\times2N$ determinant det($2\mathbf{B}$). This turns out to be not such an impossible task as might be suspected at first sight. The regular structure of the determinant allows its reduction by elementary operations to a 4×4 determinant, which is given in the appendix. For those readers who are interested in redoing the calculation we give a brief description of the procedure. Multiply the first row of the determinant by $\exp(-i\lambda_1 n)$, the second by $\exp(i\lambda_1 n)$, the third by $\exp(-i\lambda_2 n)$, the fourth by $\exp(i\lambda_2 n)$, etc, the first column by $\exp(i\lambda_1 n)$, the second by $\exp(-i\lambda_1 n)$,etc, to obtain a structure displaying the dependence of the result on $n-m$ only. Then subtract the first column from all other odd ones, the second from all other even ones. Apply a similar multiplication scheme with the factors $\exp[i\lambda_1(n-m)]$, $\exp[-i\lambda_1(n-m)]$, $\exp[i\lambda_2(n-m)]$, $\exp[-i\lambda_2(n-m)]$, ..., to the rows and with their complex conjugates to the columns. Subtracting the third row now from all odd ones and the fourth from all even ones results in a determinant with a diagonal subblock in the rows and columns 5 to $2N$. By subtracting appropriate multiples of these rows from rows 1 to 4, one obtains a factorisable problem yielding a non-trivial 4×4 determinant and a trivial $(2N-4)\times(2N-4)$ one.

We end up with a simple formula

$$\det(2\mathbf{B}) = [1+2d_\gamma(s_0^2-s_0-s_r^2)]^2 \prod_\lambda e_\lambda^2 \tag{36a}$$

with

$$r \equiv n-m \qquad s_k = \frac{1}{N}\sum_\lambda (n_\lambda+1)\,e^{i\lambda k} \qquad k \text{ any lattice vector.} \tag{36b}$$

In writing down (36) we have assumed that $s_r = s_{-r}$, i.e. $n_\lambda = n_{-\lambda}$. It is no problem to obtain the result for the more general case which, however, does not seem to have physical applications.

When we insert (36) into (35), the square root of the product over λ cancels with the partition function and we obtain

$$\langle \theta_n^+\theta_m\rangle = \{1+2\sinh^2\gamma[1+2(s_0^2-s_0-s_r^2)]\}^{-1}. \tag{37}$$

We compare this result with two limiting cases from the literature. In the dimer case, $N=2$, and

$$s_0 = \tfrac{1}{2}(n_+ + n_-)+1 \qquad s_1 = \tfrac{1}{2}(n_+ - n_-) \tag{38}$$

so that we recover the exact result of Silbey and Munn [10]:

$$\langle \theta_1^+\theta_2\rangle = \{1+2\sinh^2\gamma[n_+n_- + (n_+ +1)(n_- +1)]\}^{-1}. \tag{39}$$

Furthermore, if we write out the factor of $2\sinh^2\gamma$ in (37), we obtain

$$1+2(s_0^2-s_0-s_{n-m}^2) = \frac{1}{N^2}\sum_{\lambda\lambda'}[n_\lambda n_{\lambda'} + (n_\lambda+1)(n_{\lambda'}+1)][1-\cos(\lambda+\lambda')(n-m)]$$

$$= -\tfrac{1}{4}\langle C^2\rangle \tag{40a}$$

where

$$C = b_n^2 - b_n^{+2} - b_m^2 + b_m^{+2} \tag{40b}$$

(see [10]). It is then obvious that our result

$$\langle \theta_n^+\theta_m\rangle = (1-\tfrac{1}{2}\sinh^2\gamma\langle C^2\rangle)^{-1} \tag{41}$$

agrees to second order in γ with the approximate expression

$$\langle \theta_n^+\theta_{n+1}\rangle = (1-\gamma^2\langle C^2\rangle + \tfrac{1}{4}\gamma^4\langle C^2\rangle^2)^{-1/2} \tag{42}$$

derived by Munn and Silbey.

To conclude the discussion of this average we remark that we might possibly have derived this result with the matrix method of [11], which also involves the calculation of determinants, *provided that the determinants which occur are as tractable as the one considered here.*

Our next example, however, can in no way be treated with that method. It is obvious that, having calculated $\langle\theta_n^+\theta_m\rangle$, we can also obtain an exact formula for $\langle\theta_n^+\psi_n^+\psi_m\theta_m\rangle$, $n\neq m$, where

$$\psi_n=\exp\left(\frac{1}{\sqrt{N}}\sum_\lambda \exp(-\mathrm{i}\lambda n)Q_\lambda(b_\lambda-b_{-\lambda}^+)\right)\qquad Q_\lambda=Q_{-\lambda}^*. \tag{43}$$

The reason is that once we know how to reduce det $2\mathbf{B}$ to a 4×4 determinant, we can apply the same method to reduce det $2\mathbf{D}$ to a 5×5 determinant regardless of what the additional row and column in $\mathbf{D}$ look like. We just give a few steps of the calculation and the result. The ordered form of the average is

$$\begin{aligned}\langle\theta_n^+\psi_n^+\psi_m\theta_m\rangle=&\frac{1}{Z}\frac{1}{\cosh 2\gamma}\exp[-(q_0-q_r)^2(2+\bar{e}_r)+p_0-p_r]\\ &\times\mathrm{Tr}\Bigg[\exp\Bigg(-\frac{1}{\sqrt{N}}\sum_\lambda\{Q_\lambda[\exp(-\mathrm{i}\lambda n)-\exp(-\mathrm{i}\lambda m)]\\ &-(q_0-q_r)e_\lambda\exp(-\mathrm{i}\lambda n)\}b_\lambda\Bigg)\\ &\times\exp\left(\frac{1}{2N}t_\gamma\sum_{\lambda\lambda'}\{\exp[-\mathrm{i}(\lambda+\lambda')n]-\exp[-\mathrm{i}(\lambda+\lambda')m]\}b_\lambda b_{\lambda'}\right)\\ &\times\sum_{l,j}\frac{d_\gamma^l}{l!}\frac{d_\gamma^j}{j!}\left(\frac{1}{\sqrt{N}}\sum_{\lambda'}\exp(-\mathrm{i}\lambda' n)b_{\lambda'}\right)^l\left(\frac{1}{\sqrt{N}}\sum_{\lambda'}\exp(-\mathrm{i}\lambda' m)b_{\lambda'}\right)^j\\ &\times\left(\frac{1}{\sqrt{N}}\sum_\lambda\exp(\mathrm{i}\lambda n)b_\lambda^+\right)^l\left(\frac{1}{\sqrt{N}}\sum_\lambda\exp(\mathrm{i}\lambda m)b_\lambda^+\right)^j\\ &\times\exp\left(-\frac{1}{2N}t_\gamma\sum_{\lambda\lambda'}\{\exp[\mathrm{i}(\lambda+\lambda')n]-\exp[\mathrm{i}(\lambda+\lambda')m]\}b_\lambda^+b_{\lambda'}^+\right)\\ &\times\exp\Bigg(\frac{1}{\sqrt{N}}\sum_\lambda\{Q_{-\lambda}[\exp(\mathrm{i}\lambda n)-\exp(\mathrm{i}\lambda m)]\\ &+(q_0-q_r)e_\lambda\exp(\mathrm{i}\lambda m)\}b_\lambda^+\Bigg)\exp\left(-\sum_\lambda\beta\hbar\omega_\lambda b_\lambda^+b_\lambda\right)\Bigg]\end{aligned}\tag{44a}$$

where

$$\begin{aligned}&q_k=\frac{1}{N}\sum_\lambda Q_\lambda\exp(\mathrm{i}\lambda k)\qquad && p_k=\frac{1}{N}\sum_\lambda|Q_\lambda|^2\exp(\mathrm{i}\lambda k)\\ &\bar{e}_k=\frac{1}{N}\sum_\lambda e_\lambda\exp(\mathrm{i}\lambda k)\qquad && k\text{ lattice vector}\end{aligned}\tag{44b}$$

and e_λ is given in (33*b*). In equation (44), we have assumed $q_k=q_{-k}$, $p_k=p_{-k}$ and $\bar{e}_k=\bar{e}_{-k}$. Again, it is not difficult to write down the more general case, but since the theory in need of these averages was developed for Bravais lattices only, inversion symmetry holds and therefore $Q_\lambda=Q_{-\lambda}$.

To arrive at (44) we had to remove the linear exponentials from their position between θ_n^+ and θ_m to be able to use formulae (30) and (31) for the ordering of $\theta_n^+\theta_m$. This operation is best done in site representation with special consideration of the $b_n^{(+)}$ and $b_m^{(+)}$ terms which we commuted with θ_m and θ_n^+, respectively, whereas for all other sites the b terms are commuted in front of θ_n^+ and the b^+ terms behind θ_m. Then the cyclic property of the trace is used to obtain the b_n and b_m terms in the right order which also involves commutation with the density operator.

From (44), proceeding further is straightforward. Since all information about the occurring integrals can be inferred from the matrix **D**, we can restrict ourselves to giving this quantity. **D** is the matrix with the structure indicated in (23b), with **B** given in (34) and

$$z^{\mathrm{T}} = (z_{\lambda_1}^{\mathrm{T}}, z_{\lambda_2}^{\mathrm{T}}, \ldots, z_{\lambda_N}^{\mathrm{T}}) \tag{45a}$$

$$z_\lambda = \begin{pmatrix} \dfrac{1}{\sqrt{N}}\{Q_{-\lambda}[\exp(\mathrm{i}\lambda n) - \exp(\mathrm{i}\lambda m)] + (q_0 - q_r)e_\lambda \exp(\mathrm{i}\lambda m)\} \\ -\dfrac{1}{\sqrt{N}}\{Q_\lambda[\exp(-\mathrm{i}\lambda n) - \exp(-\mathrm{i}\lambda m)] - (q_0 - q_r)e_\lambda \exp(-\mathrm{i}\lambda n)\} \end{pmatrix}. \tag{45b}$$

The 5×5 determinant, obtained from breaking down the determinant of 2**D** in the same manner as that of 2**B** before, is again given in the appendix.

Evaluating this determinant gives the final result

$$\begin{aligned}\langle\theta_n^+\psi_n^+\psi_m\theta_m\rangle &= \frac{1}{1+2\sinh^2\gamma[1+2(s_0^2-s_0-s_r^2)]}\exp[-(p_0'-p_r'+\bar{p}_0-\bar{p}_r)] \\ &\times\exp\bigg(\frac{2\sinh\gamma}{1+2\sinh^2\gamma[1+2(s_0^2-s_0-s_r^2)]} \\ &\times\{2\sinh\gamma[(2s_0-1-2s_r)(q_0'-q_r')(\bar{q}_0-\bar{q}_r) \\ &+ s_r(q_0'-q_r'+\bar{q}_0-\bar{q}_r)^2] + \cosh\gamma(\bar{q}_0-\bar{q}_r-q_0'+q_r')(q_0'-q_r'+\bar{q}_0-\bar{q}_r)\}\bigg)\end{aligned} \tag{46a}$$

where

$$\begin{aligned} p_k' &= \frac{1}{N}\sum_\lambda |Q_\lambda|^2 n_\lambda \exp(\mathrm{i}\lambda k) & \bar{p}_k &= \frac{1}{N}\sum_\lambda |Q_\lambda|^2(n_\lambda+1)\exp(\mathrm{i}\lambda k) & &= p_k' + p_k \\ q_k' &= \frac{1}{N}\sum_\lambda Q_\lambda n_\lambda \exp(\mathrm{i}\lambda k) & \bar{q}_k &= \frac{1}{N}\sum_\lambda Q_\lambda(n_\lambda+1)\exp(\mathrm{i}\lambda k) & &= q_k' + q_k. \end{aligned} \tag{46b}$$

It is difficult to find reasonable special cases of this in the literature, against which it can be checked. Of course, setting $\gamma = 0$ reproduces the correct result for $\langle\psi_n^+\psi_m\rangle$. Also, the case $N = 2$ with $\omega_+ = \omega_-$ can be checked with the help of our introductory example.

To demonstrate another useful feature of our method we consider one final example, namely the correlation function

$$\langle\theta_{n'}^+(t)\theta_{m'}(t)\theta_n^+\theta_m\rangle = \frac{1}{Z}\mathrm{Tr}(\theta_{n'}^+\theta_{m'}\exp[-(\mathrm{i}/\hbar)Ht]\theta_n^+\theta_m\exp\{[-\beta+(\mathrm{i}/\hbar)t]H\}). \tag{47}$$

Since here the site representation operators occur in two groups separated by two groups of momentum representation diagonal operators, it would be very tedious, if not impossible, to order the whole expression. It turns out, however, that our method also works with *partial ordering*, if we use not just *one* complete set of many-particle states in the occupation number and coherent state representations but as *many* as necessary, in this case two sets of each.

First, we employ (30) and (31) to antinormally order $\theta_{n'}^{+}\theta_{m'}$ and $\theta_n^{+}\theta_m$. It is the present case, where a judicious choice has to be made whether antinormal or normal ordering is taken, since now it is no longer possible to switch from one ordering to the other by using the cyclic property of the trace. Because normal ordering would require moving the momentum representation operators between the creation and destruction parts of the site representation operators, antinormal ordering is clearly preferable.

Having ordered $\theta_{n'}^{+}\theta_{m'}$ and $\theta_n^{+}\theta_m$, we transform to momentum representation and insert complete sets of the appropriate states in the appropriate places. This results in

$$
\begin{aligned}
\langle\theta_{n'}^{+}(t)\theta_{m'}(t)\theta_n^{+}\theta_m\rangle = {} & \frac{1}{Z\cosh^2 2\gamma}\,\frac{1}{\pi^{2N}}\int\prod_\lambda \mathrm{d}^2\alpha_\lambda\int\prod_\lambda \mathrm{d}^2\beta_\lambda \sum_{\{n_\lambda\},\{m_\lambda\}} \\
& \times\left\langle\{m_\lambda\}\right|\exp\left(\frac{1}{2N}t_\gamma\sum_{\lambda,\lambda'}\{\exp[-\mathrm{i}(\lambda+\lambda')n']-\exp[-\mathrm{i}(\lambda+\lambda')m']\}\alpha_\lambda\alpha_{\lambda'}\right) \\
& \times\sum_{l,j}\frac{1}{l!}\frac{1}{j!}d_\gamma^{l}d_\gamma^{j}\left(\frac{1}{\sqrt{N}}\sum_{\lambda'}\exp(-\mathrm{i}\lambda'n')\alpha_{\lambda'}\right)^{l} \\
& \times\left(\frac{1}{\sqrt{N}}\sum_{\lambda'}\exp(-\mathrm{i}\lambda'm')\alpha_{\lambda'}\right)^{j}\left|\{\alpha_\lambda\}\right\rangle \\
& \times\left\langle\{\alpha_\lambda\}\right|\left(\frac{1}{\sqrt{N}}\sum_{\lambda}\exp(\mathrm{i}\lambda n')\alpha_\lambda^*\right)^{l}\left(\frac{1}{\sqrt{N}}\sum_{\lambda}\exp(\mathrm{i}\lambda m')\alpha_\lambda^*\right)^{j} \\
& \times\exp\left(-\frac{1}{2N}t_\gamma\sum_{\lambda,\lambda'}\{\exp[\mathrm{i}(\lambda+\lambda')n']-\exp[\mathrm{i}(\lambda+\lambda')m']\}\alpha_\lambda^*\alpha_{\lambda'}^*\right)\left|\{n_\lambda\}\right\rangle \\
& \times\left\langle\{n_\lambda\}\right|\exp\left(-\mathrm{i}t\sum_\lambda\omega_\lambda n_\lambda\right)\exp\left(\frac{1}{2N}t_\gamma\sum_{\lambda,\lambda'}\{\exp[-\mathrm{i}(\lambda+\lambda')n]\right. \\
& \left.-\exp[-\mathrm{i}(\lambda+\lambda')m]\}\beta_\lambda\beta_{\lambda'}\right) \\
& \times\sum_{l,j}\frac{1}{l!}\frac{1}{j!}d_\gamma^{l}d_\gamma^{j}\left(\frac{1}{\sqrt{N}}\sum_{\lambda'}\exp(-\mathrm{i}\lambda'n)\beta_{\lambda'}\right)^{l}\left(\frac{1}{\sqrt{N}}\sum_{\lambda'}\exp(-\mathrm{i}\lambda'm)\beta_{\lambda'}\right)^{j}\left|\{\beta_\lambda\}\right\rangle \\
& \times\left\langle\{\beta_\lambda\}\right|\left(\frac{1}{\sqrt{N}}\sum_{\lambda}\exp(\mathrm{i}\lambda n)\beta_\lambda^*\right)^{l}\left(\frac{1}{\sqrt{N}}\sum_{\lambda}\exp(\mathrm{i}\lambda m)\beta_\lambda^*\right)^{j} \\
& \times\exp\left(-\frac{1}{2N}t_\gamma\sum_{\lambda,\lambda'}\{\exp[\mathrm{i}(\lambda+\lambda')n]-\exp[\mathrm{i}(\lambda+\lambda')m]\}\beta_\lambda^*\beta_{\lambda'}^*\right) \\
& \times\exp\left((\mathrm{i}t-\beta\hbar)\sum_\lambda\omega_\lambda m_\lambda\right)\left|\{m_\lambda\}\right\rangle. \qquad (48)
\end{aligned}
$$

Herein, the m_λ and n_λ are occupation numbers, whereas α_λ and β_λ are eigenvalues of b_λ in the coherent states $|\alpha_\lambda\rangle$ and $|\beta_\lambda\rangle$, respectively. Even in (48) the sums over occupation numbers can be performed. Instead of (10), we use

$$\sum_\lambda \langle\alpha\,|\,n\rangle\langle n\,|\,\beta\rangle e^{-dn} = \sum_n \exp[-\tfrac{1}{2}(|\alpha|^2+|\beta|^2)]\frac{(\alpha^*\beta e^{-d})^n}{n!}$$
$$= \exp[-\tfrac{1}{2}(\alpha^*\alpha+\beta^*\beta)]\exp(\alpha^*\beta e^{-d}). \tag{49}$$

It is then obvious that the integrand again takes the form $\exp\{-\boldsymbol{\alpha}^+\mathbf{B}\boldsymbol{\alpha}\}$, where now $\mathbf{B}$ is a $4N\times 4N$ matrix and

$$\boldsymbol{\alpha}^+ = (\alpha^*_{\lambda_1}, \alpha_{\lambda_1}, \alpha^*_{\lambda_2}, \alpha_{\lambda_2}, \ldots, \alpha_{\lambda_N}, \beta^*_{\lambda_1}, \beta_{\lambda_1}, \beta^*_{\lambda_2}, \ldots, \beta_{\lambda_N}) \tag{50}$$

is a $4N$ vector.

The matrix $\mathbf{B}$ is composed of four $2N\times 2N$ blocks:

$$\mathbf{B} = \begin{pmatrix} \mathbf{B}^{\alpha\alpha} & \mathbf{B}^{\alpha\beta} \\ \mathbf{B}^{\beta\alpha} & \mathbf{B}^{\beta\beta} \end{pmatrix} \qquad \mathbf{B}^{\rho\sigma} = \begin{pmatrix} \mathbf{B}^{\rho\sigma}_{\lambda_1\lambda_1} & \cdots & \mathbf{B}^{\rho\sigma}_{\lambda_1\lambda_N} \\ \vdots & & \vdots \\ \mathbf{B}^{\rho\sigma}_{\lambda_N\lambda_1} & \cdots & \mathbf{B}^{\rho\sigma}_{\lambda_N\lambda_N} \end{pmatrix} \qquad \rho, \sigma = \alpha, \beta \tag{51a}$$

with

$$\mathbf{B}^{\alpha\alpha}_{\lambda\lambda'} = \frac{1}{2}\begin{bmatrix} \delta_{\lambda\lambda'} - \dfrac{d_\gamma}{N}\{\exp[\mathrm{i}(\lambda-\lambda')n'] + \exp[\mathrm{i}(\lambda-\lambda')m']\} & \dfrac{t_\gamma}{N}\{\exp[\mathrm{i}(\lambda+\lambda')n'] - \exp[\mathrm{i}(\lambda+\lambda')m']\} \\ -\dfrac{t_\gamma}{N}\{\exp[-\mathrm{i}(\lambda+\lambda')n'] - \exp[-\mathrm{i}(\lambda+\lambda')m']\} & \delta_{\lambda\lambda'} - \dfrac{d_\gamma}{N}\{\exp[-\mathrm{i}(\lambda-\lambda')n'] + \exp[-\mathrm{i}(\lambda-\lambda')m']\} \end{bmatrix} \tag{51b}$$

and $\mathbf{B}^{\beta\beta}_{\lambda\lambda'}$ the same matrix with n', m' replaced by n and m, respectively. The two remaining blocks are given by

$$\mathbf{B}^{\alpha\beta}_{\lambda\lambda'} = \frac{1}{2}\begin{pmatrix} -g_\lambda\delta_{\lambda\lambda'} & 0 \\ 0 & -f_\lambda\delta_{\lambda\lambda'} \end{pmatrix}$$
$$\mathbf{B}^{\beta\alpha}_{\lambda\lambda'} = \frac{1}{2}\begin{pmatrix} -f_\lambda\delta_{\lambda\lambda'} & 0 \\ 0 & -g_\lambda\delta_{\lambda\lambda'} \end{pmatrix} \tag{51c}$$

where

$$f_\lambda = \exp[(\mathrm{i}t-\beta\hbar)\omega_\lambda] \qquad g_\lambda = \exp(-\mathrm{i}t\omega_\lambda). \tag{51d}$$

Using the same procedure as in the first example of this section we can reduce the $4N\times 4N$ determinant of $2\mathbf{B}$ to an 8×8 determinant. This calculation, though trivial, is very tedious. To make it feasible in a reasonable amount of time, we used the symbol manipulation program SMP†. It turns out that the resulting 8×8 determinant can immediately be simplified to a 4×4 one. This determinant is also given in the appendix. For the general case, it is probably the most compact form of the result, since its expanded form is a lengthy expression. Therefore, this formula shall not be reproduced

† The program was developed by Stephen Wolfram. Copyright © 1983, Inference Corporation.

here and we consider the special cases $n'=m$, $m'=n$ and $n'=n$, $m'=m$ only, leading to much simpler formulae. These are given by

$$\langle\theta_m^+(t)\theta_n(t)\theta_n^+\theta_m\rangle = T_- \tag{52a}$$

$$\langle\theta_n^+(t)\theta_m(t)\theta_n^+\theta_m\rangle = T_+ \tag{52b}$$

where

$$\begin{aligned}T_\mp = (1 + 4\sinh^2\gamma\cosh^2\gamma[1+2(s_0^2 - s_0 - s_r^2) \mp (f_0^2 - f_r^2 + g_0^2 - g_r^2)] \\ + \sinh^4\gamma\{-1+16[(s_0 - \tfrac{1}{2} - s_r)^2 - (f_0 - f_r)(g_0 - g_r)] \\ \times[(s_0 - \tfrac{1}{2} + s_r)^2 - (f_0 + f_r)(g_0 + g_r)]\})^{-1}\end{aligned} \tag{52c}$$

with

$$f_k = \frac{1}{N}\sum_\lambda n_\lambda \exp(\mathrm{i}\omega_\lambda t)\exp(\mathrm{i}\lambda k) \qquad g_k = \frac{1}{N}\sum_\lambda (n_\lambda+1)\exp(-\mathrm{i}\omega_\lambda t)\exp(\mathrm{i}\lambda k). \tag{52d}$$

f_k and g_k are the Fourier transforms of f_λ/e_λ and g_λ/e_λ, respectively. r, s_0 and s_r are defined as in (36b).

Although slightly more complicated, the explicit version of this expression seems somewhat more transparent:

$$\begin{aligned}T_\mp = \Bigg\{1 + 4\sinh^2\gamma\cosh^2\gamma\frac{1}{N^2}\sum_{\lambda\lambda'}(n_\lambda n_{\lambda'}\{1\mp\exp[\mathrm{i}(\omega_\lambda+\omega_{\lambda'})t]\} \\ +(n_\lambda+1)(n_{\lambda'}+1)\{1\mp\exp[-\mathrm{i}(\omega_\lambda+\omega_{\lambda'})t]\})[1-\cos(\lambda+\lambda')r] \\ +\sinh^4\gamma\Bigg[-1+\Bigg(1-\frac{4}{N^2}\sum_{\lambda\lambda'}n_\lambda(n_{\lambda'}+1)\{1-\exp[\mathrm{i}(\omega_\lambda-\omega_{\lambda'})t]\} \\ \times[1-\cos\lambda r-\cos\lambda' r+\cos(\lambda+\lambda')r]\Bigg) \\ \times\Bigg(1-\frac{4}{N^2}\sum_{\lambda\lambda'}n_\lambda(n_{\lambda'}+1)\{1-\exp[\mathrm{i}(\omega_\lambda-\omega_{\lambda'})t]\} \\ \times[1+\cos\lambda r+\cos\lambda' r+\cos(\lambda+\lambda')r]\Bigg)\Bigg]\Bigg\}^{-1}.\end{aligned} \tag{53}$$

Specialising once again to the case $N=2$, we see that the summands in the $\sinh^4\gamma$ term vanish for $\lambda=\lambda'$ because of the time factor and for $\lambda\neq\lambda'$ because of the space factor (containing $\cos\lambda r$, etc). This eliminates the whole $\sinh^4\gamma$ term and we are left with

$$\begin{aligned}T_\mp = [1+\sinh^2 2\gamma(n_+n_-\{1\mp\exp[\mathrm{i}(\omega_++\omega_-)t]\}+(n_++1)(n_-+1) \\ \times\{1\mp\exp[-\mathrm{i}(\omega_++\omega_-)t]\})]^{-1}.\end{aligned} \tag{54}$$

As expected, T_- coincides with the Munn–Silbey result for a dimer [10]. Furthermore T_+ at $t=0$ gives the average of $\theta_n^+\theta_m$ with γ replaced by 2γ, as it should.

However, since the terms containing frequency differences (rather than sums) cancel exactly for $N=2$, the procedure devised by Silbey and Munn [10] to obtain an approximation for $N>2$ by generalising the $N=2$ result fails to account for these terms. They are of order γ^4 and higher as our exact result shows. Therefore, only the γ^2 terms are correctly reproduced by the procedure in [10].

4. Conclusions

The method introduced here provides a relatively easy route to the evaluation of thermal averages of exponential quadratic phonon operators. In particular, we have been able to evaluate a number of averages which Munn and Silbey [10] introduced and were unable to evaluate in their work on quadratic electron–phonon interactions. Thus, this method is a powerful approach to these averages and is a useful addition to the list of techniques for evaluating these [11].

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Appendix

First, we give the result of the reduction of det 2**D** to a 5×5 determinant in the calculation of $\langle\theta_n^+\psi_n^+\psi_m\theta_m\rangle$:

$$\det 2\mathbf{D}=\left(\prod_\lambda e_\lambda^2\right)\begin{vmatrix} \begin{matrix}4(\bar p_0-\bar p_r)\\-2(q_0-q_r)^2(2+\bar e_r)\end{matrix} & \begin{matrix}-d_\gamma(q_0'-q_r')\\+t_\gamma(\bar q_0-\bar q_r)\end{matrix} & \begin{matrix}d_\gamma(\bar q_0-\bar q_r)\\+t_\gamma(q_0'-q_r')\end{matrix} & \bar q_0-\bar q_r & -q_0'+q_r' \\ \bar q_0-\bar q_r & 1-d_\gamma s_0 & t_\gamma s_0 & -s_r & 0 \\ -q_0'+q_r' & -t_\gamma s_0 & 1-d_\gamma s_0 & 0 & -s_r \\ \begin{matrix}-d_\gamma(q_0'-q_r')\\+t_\gamma(\bar q_0-\bar q_r)\end{matrix} & -2d_\gamma s_r & 0 & 1-d_\gamma s_0 & -t_\gamma s_0 \\ \begin{matrix}d_\gamma(\bar q_0-\bar q_r)\\+t_\gamma(q_0'-q_r')\end{matrix} & 0 & -2d_\gamma s_r & t_\gamma s_0 & 1-d_\gamma s_0 \end{vmatrix} \tag{A1}$$

The determinant of 2**B** for this problem *and* for the calculation of $\langle\theta_n\theta_m^+\rangle$ is obtained by crossing out the first row and column (and keeping the prefactors). The quantities appearing in this determinant are explained in (36*b*), (44*b*) and (46*b*).

It may be mentioned that the <u>11</u> element of this determinant leads to a partial cancellation of the exponential prefactor in (44*a*), making the result independent of $\bar e_r$. This is reasonable as it preserves the symmetric occurrence of n_λ and $n_\lambda+1$ in the final formula. (Notice that $s_r=(1/N)\,\Sigma_\lambda\,(n_\lambda+1)\,e^{i\lambda r}=(1/N)\,\Sigma_\lambda\,n_\lambda\,e^{i\lambda r}$ for $r\neq0$.)

The general result of our third example is given by

$$\langle\theta_{n'}^+(t)\theta_{m'}(t)\theta_n^+\theta_m\rangle=\frac{1}{Z\cosh^2 2\gamma}\frac{1}{(\det 2\mathbf{B})^{1/2}} \tag{A2}$$

with

$$\det 2\mathbf{B} = (2d_\gamma)^4\left(\prod_\lambda e_\lambda^2\right)$$
$$\times\begin{vmatrix} \begin{array}{l}-\bar{s}_0^2+s_{r'}^2-(t_\gamma/2d_\gamma)^2\\ -g_p^2+g_{p+r}^2\end{array} & g_{p'}g_{p+r}-g_pg_{p-r'} & \begin{array}{l}-\bar{s}_0(f_p+g_p)\\ +f_{p-r'}s_{r'}+g_{p+r}s_r\end{array} & \begin{array}{l}-\bar{s}_0(f_{p+r}-g_{p+r})\\ +f_{p'}s_{r'}-g_ps_r\end{array} \\ g_{p'}g_{p+r}-g_pg_{p-r'} & \begin{array}{l}\bar{s}_0^2-s_{r'}^2+(t_\gamma/2d_\gamma)^2\\ +g_{p'}^2-g_{p-r'}^2\end{array} & \begin{array}{l}\bar{s}_0(f_{p-r'}-g_{p-r'})\\ -f_ps_{r'}+g_{p'}s_r\end{array} & \begin{array}{l}\bar{s}_0(f_{p'}+g_{p'})\\ -f_{p+r}s_{r'}+g_{p-r'}s_r\end{array} \\ \begin{array}{l}-s_0(f_p+g_p)\\ +f_{p-r'}s_{r'}+g_{p+r}s_r\end{array} & \begin{array}{l}\bar{s}_0(f_{p-r'}-g_{p-r'})\\ +g_{p'}s_r-f_ps_{r'}\end{array} & \begin{array}{l}-\bar{s}_0^2+s_r^2-(t_\gamma/2d_\gamma)^2\\ -f_p^2+f_{p-r}^2\end{array} & f_{p'}f_{p-r'}-f_pf_{p+r} \\ \begin{array}{l}-\bar{s}_0(f_{p+r}-g_{p+r})\\ +f_{p'}s_{r'}-g_ps_r\end{array} & \begin{array}{l}\bar{s}_0(f_{p'}+g_{p'})\\ -f_{p+r}s_{r'}+g_{p-r'}s_r\end{array} & f_{p'}f_{p-r'}-f_pf_{p+r} & \begin{array}{l}\bar{s}_0^2-s_r^2+(t_\gamma/2d_\gamma)^2\\ +f_{p'}^2-f_{p+r}^2\end{array} \end{vmatrix} \tag{A3}$$

where $\bar{s}_0 = s_0 - \frac{1}{2}$, $r' = n' - m'$, $r = n - m$, $p = n' - n$, $p' = m' - m$, and the other quantities are explained in (36b) and (52d).

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