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Thermal averages for the harmonic oscillator: an extension of Bloch's 'second' theorem

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Abstract. The thermal average of $\exp\{f(q, p)\}$ is given by Bloch's 'second' theorem when f is an arbitrary linear function of q and p. Formulae are presented here for when f is a quadratic form. In contrast to linear f, there are different cases to be considered depending on the coefficients of the quadratic form. A new complete orthonormal set of functions proves useful in evaluating the averages and is given in the appendix.

1. Introduction

A frequently encountered average in the scattering of waves in condensed systems is the average $\langle\ \rangle_0$ of the operator $\exp(a_1 b + a_2 b^+)$ taken with respect to the thermal equilibrium distribution of a simple harmonic oscillator at temperature $T = (k_B\beta)^{-1}$. It is given by Bloch's 'second' theorem [1]:

$$\langle\exp(a_1 b + a_2 b^+)\rangle_0 = \exp\{\tfrac{1}{2}\langle(a_1 b + a_2 b^+)^2\rangle_0\} = \exp\{\tfrac{1}{2}a_1 a_2 \coth(\beta/2)\}. \qquad (1)$$

The oscillator frequency ω has been set equal to one, and

$$b = 2^{-1/2}(q + \mathrm{i}p) \qquad b^+ = 2^{-1/2}(q - \mathrm{i}p)$$

are boson operators, while a_1, a_2 are arbitrary coefficients. In this paper we derive parallel formulae for the harmonic average of quadratic exponentials. In the derivation use is made of an apparently new complete orthonormal set of functions which are the eigenfunctions of the operator

$$\mathscr{L} = qp + pq. \qquad (2)$$

The particular average $\langle\exp\{\mathrm{i}\lambda p\}\rangle_0$ appears in the small-polaron problem as a renormalisation factor, after a canonical transformation, multiplying the matrix element for the hopping of an electron between neighbouring sites in the presence of linear coupling ($\propto q$) to a phonon mode [2]. The average, $\langle\exp \mathrm{i}k\mathscr{L}\rangle_0$, arises in a similar manner when the coupling is quadratic, i.e. $\propto q^2$ [3].

2. Quadratic forms

The general form of second order in b and b^+ is a linear combination of the following three Hermitian operators:

$$U = \tfrac{1}{2}(b^+ b + b b^+) = \tfrac{1}{2}(q^2 + p^2) \qquad (3a)$$

$$V_1 = (1/2\mathrm{i})(b^2 - b^{+2}) = \tfrac{1}{2}(qp + pq) = \tfrac{1}{2}\mathscr{L} \qquad (3b)$$

$$V_2 = \tfrac{1}{2}(b^2 + b^{+2}) = \tfrac{1}{2}(q^2 - p^2). \qquad (3c)$$

The first is the oscillator Hamiltonian ($\omega \equiv 1$). It has a discrete spectrum and is bounded from below, while the other two are unbounded both above and below with continuous spectra consisting of the entire interval $(-\infty, \infty)$. Therefore, unlike in equation (1), restrictions must be imposed on the coefficients in the second order form:

$$Q(a', b_1', b_2') = a'U + b_1' V_1 + b_2' V_2 \tag{4}$$

in order for the average $\langle \exp Q \rangle_0$ to exist. We will assume in what follows that the ratios $a' : b_1' : b_2'$ are real and will write

$$Q(\alpha, a, b_1, b_2) = -\alpha(aU + b_1 V_1 + b_2 V_2) \tag{4'}$$

where a, b_1 and b_2 are real; $a \geqslant 0$ and $|\alpha| = 1$.

The operators (3) have the commutators

$$[U, V_1] = 2\mathrm{i} V_2 \tag{5a}$$

$$[V_1, V_2] = -2\mathrm{i} U \tag{5b}$$

$$[U, V_2] = -2\mathrm{i} V_1 . \tag{5c}$$

These are the same as for the generators of the Lorentz group in 2+1 dimensions, with $U/2$ generating the 2-space rotations and $V_1/2$, $V_2/2$ generating the Lorentz 'boosts'. They form an invariant

$$V_1^2 + V_2^2 - U^2 = \tfrac{3}{4} \tag{6}$$

under the rotation and boost operators

$$R(\theta) = \exp(-\mathrm{i}\theta U/2) \tag{7a}$$

$$L_1(\eta) = \exp(\mathrm{i}\eta V_1/2) \tag{7b}$$

$$L_2(\zeta) = \exp(-\mathrm{i}\zeta V_2/2) \tag{7c}$$

respectively, and we have the transformations

$$\begin{pmatrix} U(\theta) \\ V_1(\theta) \\ V_2(\theta) \end{pmatrix} = R^{-1}(\theta) \begin{pmatrix} U \\ V_1 \\ V_2 \end{pmatrix} R(\theta) = \begin{pmatrix} U \\ V_1 \cos\theta - V_2 \sin\theta \\ V_1 \sin\theta + V_2 \cos\theta \end{pmatrix} \tag{8a}$$

$$\begin{pmatrix} U(\eta) \\ V_1(\eta) \\ V_2(\eta) \end{pmatrix} = L_1^{-1}(\eta) \begin{pmatrix} U \\ V_1 \\ V_2 \end{pmatrix} L_1(\eta) = \begin{pmatrix} U \cosh\eta - V_2 \sinh\eta \\ V_1 \\ -U \sinh\eta + V_2 \cosh\eta \end{pmatrix} \tag{8b}$$

$$\begin{pmatrix} U(\zeta) \\ V_1(\zeta) \\ V_2(\zeta) \end{pmatrix} = L_2^{-1}(\zeta) \begin{pmatrix} U \\ V_1 \\ V_2 \end{pmatrix} L_2(\zeta) = \begin{pmatrix} U \cosh\zeta - V_1 \sinh\zeta \\ -U \sinh\zeta + V_1 \cosh\eta \\ V_2 \end{pmatrix} . \tag{8c}$$

3. Calculations

The average of $\exp Q$ has the form

$$\langle \exp Q \rangle_0 = 2 \sinh(\beta/2) I \tag{9}$$

where

$$I = \mathrm{Tr}\{\exp(-\beta U) \exp Q\} \tag{10}$$

and

$$2\sinh(\beta/2) = (\mathrm{Tr}\exp(-\beta U))^{-1}.$$

Through use of the rotation equation ($8a$), the coefficient of either V_1 or V_2 in Q may be made zero so that either

$$Q' = -\alpha(aU + bV_1) \tag{11a}$$

or

$$\begin{aligned} Q'' &= -\alpha(aU + bV_2) \\ &= -\alpha[(a-b)p^2 + (a+b)q^2]/2 \end{aligned} \tag{11b}$$

may be used in (10) without changing its value, where $b = \pm(b_1^2 + b_2^2)^{1/2}$ in ($11a$) and ($11b$), respectively. The form multiplying α in Q'' is clearly bounded from below when $a > |b|$ and unbounded on both sides for $a < |b|$. These two cases will be considered separately.

3.1. $a > |b|$

$$Q'' = -\alpha(cp^2 + dq^2)/2 \tag{12}$$

where $c = a - b$, $d = a + b$ are both positive. The trace will be evaluated in coordinate space, so that

$$I = \int \mathrm{d}q_1\,\mathrm{d}q_2 \langle q_1|\exp(-\beta U)|q_2\rangle\langle q_2|\exp[-\alpha(cp^2 + dq^2)/2]|q_1\rangle. \tag{13}$$

Feynman's book on statistical mechanics [4] gives (equation (2-83)) the following expression for the density matrix of an oscillator of mass m and frequency ω:

$$\begin{aligned} &\langle x_1|\exp[-\beta(p_x^2/2m + m\omega^2 x^2/2)]|x_2\rangle \\ &\quad = \left(\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}\right)^{1/2} \\ &\quad\quad \times \exp\left(-\frac{m\omega}{2\hbar\sinh(\beta\hbar\omega)}[(x_1^2 + x_2^2)\cosh(\beta\hbar\omega) - 2x_1x_2]\right). \end{aligned} \tag{14}$$

With appropriate substitutions of the above into the two integrand factors in equation (13) we obtain the integral

$$I = (d/c)^{1/4}(4\pi^2\sinh\beta\sinh\alpha\beta')^{-1/2}\int \mathrm{d}q_1\,\mathrm{d}q_2\exp[-\tfrac{1}{2}K(q_1^2 + q_2^2) - Lq_1q_2] \tag{15}$$

where $\beta' = (cd)^{1/2}$ and

$$\begin{aligned} K &= \coth\beta + (d/c)^{1/2}\coth(\alpha\beta') \\ L &= \frac{1}{\sinh\beta} + \left(\frac{d}{c}\right)^{1/2}\frac{1}{\sinh(\alpha\beta')} \end{aligned} \tag{16}$$

are, in general, complex through α. The conditions for convergence of a multiple Gaussian integral with a complex coefficient matrix A are given in appendix 2. For the above case, they are

$$\mathrm{Re}\,K \geq 0 \qquad (\mathrm{Re}\,K)^2 - (\mathrm{Re}\,L)^2 \geq 0$$

and (17)

$$\det A = (K^2 - L^2) \neq 0.$$

Then the integral in (15) is given by the familiar form

$$(4\pi^2/\det A)^{1/2} \tag{18}$$

with the result that

$$I = \{[(c/d)^{1/2} + (d/c)^{1/2}] \sinh\beta \sinh(\alpha\beta') + 2[\cosh\beta \cosh(\alpha\beta') - 1]\}^{-1/2}. \tag{19}$$

There is a symmetry with respect to β and $\alpha\beta'$ because of the oscillator form of Q'' in (12), namely $Q'' = -\alpha\beta' U(q', p')$, with $q' = (d/c)^{1/4} q$ and $p' = (c/d)^{1/4} p$. Special cases of equation (17) may be noted as follows.

(i) $c = d (= a)$ and $\beta + a \operatorname{Re} \alpha > 0$:

$$I = \operatorname{Tr}\{e^{-\beta U} e^{-\alpha a U}\} = \{2 \sinh[(\beta + \alpha a)/2]\}^{-1}.$$

(ii) $c = 0$:

$$I = \operatorname{Tr}\{e^{-\beta U} \exp(-\varepsilon q^2)\} = 2^{-1/2}(\varepsilon \sinh\beta + \cosh\beta - 1)^{-1/2}$$

as long as $\beta + \frac{1}{2}\operatorname{Re}\varepsilon \geqslant 0$. The case $d = 0$ is the same, so that

$$\langle \exp(-\varepsilon q^2)\rangle_0 = \langle \exp(-\varepsilon p^2)\rangle_0 = (1 + \varepsilon \coth\beta/2)^{-1/2}. \tag{20}$$

(iii) α pure imaginary, say, $\alpha \propto it$. Since c and d in equation (12) define the Hamiltonian H_0' for an oscillator with different mass and frequency ($c/d = (m\omega/m'\omega')^2$), equations (9) and (19) give a hybrid quantity, namely the thermal average with respect to H_0 (m, ω) of the time evolution operator belonging to $H_0'(m', \omega')$:

$$\langle \exp(-itH_0'/\hbar)\rangle_0 = \Bigg[\cos\omega' t - 2(1 - \cos\omega' t) n_0(n_0 + 1)$$
$$+ i\left(\frac{m\omega}{m'\omega'} + \frac{m'\omega'}{m\omega}\right)(n_0 + \tfrac{1}{2}) \sin\omega' t\Bigg]^{-1} \tag{21}$$

where $n_0 = (e^{\beta\hbar\omega} - 1)^{-1}$ and all the dimensional quantities are shown explicitly.

3.2. $a < |b|$

This is more involved than the previous case because Q'' in equation (11) now has the character of V_2. Using the boost transformation (8b), with

$$\eta = \ln\gamma \qquad \gamma = \left(\frac{b + a}{b - a}\right)^{1/2} \tag{22}$$

I becomes

$$\operatorname{Tr}(e^{-\beta U(\eta)} e^{-\alpha b' V_2})$$

where

$$b' = (b^2 - a^2)^{1/2} \tag{23a}$$

and

$$U(\eta) = (\gamma p^2 + \gamma^{-1} q^2)/2. \tag{23b}$$

Writing γ, which is real and positive, as $\gamma = m'/m$ shows that $\hbar\omega U(\eta)$ is the Hamiltonian for an oscillator of the same ω as U but different mass. Then

$$I = \int \mathrm{d}q_1\, \mathrm{d}q_2\, \langle q_1|c^{-\beta U(\eta)}|q_2\rangle\langle q_2|\exp(-\alpha b' V_2)|q_1\rangle \tag{24}$$

where q_1 and q_2 are dimensionless. Transcribing the first matrix element above from equation (14) gives

$$\left(\frac{\gamma}{2\pi \sinh\beta}\right)\exp\left\{-\frac{\gamma}{2}\left((q_1^2+q_2^2)\coth\beta - \frac{2q_1q_2}{\sinh\beta}\right)\right\}. \tag{25}$$

The second matrix element needs a little more work. It proves expedient to rewrite it first in terms of the corresponding matrix elements of V_1 which are derived in appendix 1. Because of the two-sided unboundedness of V_1, it is necessary to restrict α to be pure imaginary,

$$\alpha b' = \mathrm{i}\tau \qquad \tau \text{ real} \tag{26}$$

so that $\alpha = \mathrm{i}\,\mathrm{sgn}\,\tau$. The result is quasidiagonal in q:

$$\langle q|\exp(-\mathrm{i}\tau V_1)|q'\rangle = \delta(q\,\mathrm{e}^{-\tau/2} - q'\,\mathrm{e}^{\tau/2}). \tag{27}$$

Since the rotation $R(\pi/2)$ in equation ($8a$) gives $V_2(\pi/2) = V_1$, we obtain

$$\begin{aligned}\langle q_2|&\exp(\mathrm{i}\tau V_2)|q_1\rangle \\ &= \int \mathrm{d}q\,\mathrm{d}q'\langle q_2|\exp(-\mathrm{i}\pi U/4)|q\rangle\langle q'|\exp(\mathrm{i}\pi U/4)|q_1\rangle\,\mathrm{e}^{\tau/2}\delta(q-q'\,\mathrm{e}^{\tau}) \\ &= (2\pi\mathrm{i}\sinh\tau)^{-1/2}\exp\{\tfrac{1}{2}\mathrm{i}[(q_2^2+q_1^2)\coth\tau - (2q_2q_1/\sinh\tau)]\}.\end{aligned} \tag{28}$$

This has the same form as (25) except for replacing γ by $-\mathrm{i}$, but still retaining the hyperbolic functions. In comparison, the more familiar time evolution operator for an oscillator has trigonometric functions:

$$\langle q_2|\,\mathrm{e}^{-\mathrm{i}\tau U}|q_1\rangle = (2\pi\mathrm{i}\sin\tau)^{-1/2}\exp\{\tfrac{1}{2}\mathrm{i}[(q_2^2+q_1^2)\cot\tau - (2q_2q_1/\sin\tau)]\}. \tag{29}$$

Motion in the inverted potential $-q^2/2$ in V_2 is characterised by the real exponentials in equation (28). These also appear in equation (27) which involves a $\pi/4$ rotation of the phase space. (Equation (28) can be derived, without reference to V_1, by direct integration of the time dependent Schrödinger equation for the left-hand member of equation (28) following the procedure in § 2.5 in reference [4] for the Bloch equation $(\partial\rho/\partial\beta)$ for the harmonic oscillator density matrix.)

Inserting (25) and (28) into equation (24) and using (18) gives

$$I = [2(\cosh\beta\cosh\tau - 1) + \mathrm{i}(\gamma - \gamma^{-1})\sinh\beta\sinh\tau]^{-1/2}. \tag{30}$$

For the special case $a = 0$, γ is unity and

$$\langle\exp(\pm\mathrm{i}\tau V_2)\rangle_0 = \langle\exp(\pm\mathrm{i}\tau V_1)\rangle_0 = \sqrt{2}\sinh(\beta/2)(\cosh\beta\cosh\tau - 1)^{-1/2}. \tag{31}$$

The V_1 form is significant because the operator

$$\exp(\mathrm{i}\tau V_1) = \exp[\tau(b^2 - b^{+2})/2] = L(2\tau) \tag{32}$$

produces the Bogoliubov transformation of the boson operators, i.e.

$$\begin{pmatrix} b(\tau) \\ b^+(\tau)\end{pmatrix} = L^{-1}(2\tau)\begin{pmatrix} b \\ b^+\end{pmatrix}L(2\tau) = \begin{pmatrix} b\cosh\tau - b^+\sinh\tau \\ -b\sinh\tau + b^+\cosh\tau\end{pmatrix} \tag{33}$$

which mixes b and b^+, while maintaining canonical commutation relations. The averages (31) give a (mean-field) renormalisation factor for electron hopping in the case of an interacting phonon-electron system with coupling proportional to q^2 [3].

Finally, we record equations (19) and (30) in terms of the original set of coefficients:

$$\begin{aligned} I(\alpha, a, b_1, b_2; \beta) &= \mathrm{Tr}\{\exp(-\beta U)\exp[-\alpha(aU+b_1V_1+b_2V_2)]\} \\ &= \left\{\left[\left(\frac{a+(b_1^2+b_2^2)^{1/2}}{a-(b_1^2+b_2^2)^{1/2}}\right)^{1/2}+\left(\frac{a-(b_1^2+b_2^2)^{1/2}}{a+(b_1^2+b_2^2)^{1/2}}\right)^{1/2}\right]\right. \\ &\quad \times \sinh\beta\,\sinh[\alpha(a^2-b_1^2-b_2^2)^{1/2}] \\ &\quad \left. +2\{\cosh\beta\,\cosh[\alpha(a^2-b_1^2-b_2^2)^{1/2}]-1\}\right\}^{-1/2} \end{aligned} \tag{34}$$

when $a \geqslant (b_1^2+b_2^2)^{1/2}$, and

$$\begin{aligned} I(\alpha, a, b_1, b_2; \beta) &= \left\{2[\cosh\beta\,\cosh(b_1^2+b_2^2-a^2)^{1/2}-1]+\alpha\left[\left(\frac{(b_1^2+b_2^2)^{1/2}+a}{(b_1^2+b_2^2)^{1/2}-a}\right)^{1/2}\right.\right. \\ &\quad \left.\left.-\left(\frac{(b_1^2+b_2^2)^{1/2}-a}{(b_1^2+b_2^2)^{1/2}+a}\right)^{1/2}\right]\sinh\beta\,\sinh(b_1^2+b_2^2-a^2)^{1/2}\right\} \end{aligned} \tag{35}$$

when $a < (b_1^2+b_2^2)^{1/2}$ and $\alpha = \pm \mathrm{i}$. The coefficients a, b_1, b_2 are real and $a \geqslant 0$ in both cases.

Appendix 1. The eigenfunctions of $V_1 = \frac{1}{2}(qp+pq)$

The eigenvalue equation in q is

$$V_1\phi(q) = -\mathrm{i}(q\,\mathrm{d}/\mathrm{d}q+\tfrac{1}{2})\phi(q) = v\phi(q). \tag{A1.1}$$

This has normalisable solutions, in the continuum sense, of the form

$$\phi(q) = C\exp(z\ln|q|) = C|q|^{-1/2}\exp(\mathrm{i}v\ln|q|) \tag{A1.2}$$

where

$$z = \mathrm{i}v - \tfrac{1}{2}$$

and v is any *real* number. In checking (A1.2), the condition $q\delta(q) = 0$ is used. The set

$$\begin{aligned} \phi_v^+(q) &= (2\pi)^{-1/2}\theta(q)\exp(z(v)\ln q) \\ \phi_v^-(q) &= (2\pi)^{-1/2}\theta(-q)\exp(z(v)\ln(-q)) \end{aligned} \tag{A1.3}$$

is complete and orthonormal, i.e.

$$\int_{-\infty}^{\infty} \mathrm{d}q(\phi_v^\sigma(q))^*\phi_{v'}^{\sigma'}(q) = \delta_{\sigma\sigma'}\delta(v-v') \tag{A1.4}$$

where $\sigma = +, -$, and

$$\sum_\sigma \int_{-\infty}^{\infty} \mathrm{d}v\,(\phi_v^\sigma(q))^*\phi_v^\sigma(q') = \delta(q-q'). \tag{A1.5}$$

To derive equation (27), consider

$$\begin{aligned} J &= \langle q|\exp(-\alpha b V_1)|q'\rangle \\ &= \sum_\sigma \int_{-\infty}^{\infty} \mathrm{d}v\, \phi_v^\sigma(q)\phi_v^\sigma(q')\,\mathrm{e}^{-bv} \\ &= \frac{1}{2\pi}\frac{\theta(qq')}{|qq'|^{1/2}}\int_{-\infty}^{\infty}\mathrm{d}v\,\exp(\mathrm{i}v\ln|q/q'|)\exp(-\alpha b v) \end{aligned} \tag{A1.6}$$

where $|\alpha| = 1$ and $b > 0$.

Convergence of the integral requires αb to be pure imaginary. Setting $\alpha b = \mathrm{i}\tau$ gives

$$\begin{aligned} J &= \frac{\theta(qq')}{|qq'|^{1/2}}\delta(\ln|q/q'| - \tau) \\ &= \mathrm{e}^{\tau/2}\delta(q - q'\,\mathrm{e}^{\tau}). \end{aligned} \tag{A1.7}$$

Thermodynamic integrals like $\mathrm{Tr}\,\mathrm{e}^{-\beta V}$ do not exist for V_1 and V_2 because of their negative unbounded spectrum.

Appendix 2. Gaussian integrals with complex matrices

We consider the multivariate infinite integral

$$I(A) = \int \mathrm{d}^n q\, \exp\{-q^T A q\} \tag{A2.1}$$

where the q_i, $i = 1, \ldots, n$, are real variables. When the matrix A is real (A2.1) converges if A is positive, i.e. all its eigenvalues are greater than zero, and then

$$I(A) = (\pi^n/\det A)^{1/2}. \tag{A2.2}$$

We derive here the 'almost well known' generalisation for when A is complex, i.e.

$$A = B + \mathrm{i}C \tag{A2.3}$$

where B and C are real symmetric matrices. The necessary and sufficient conditions for convergence of (A2.1) are that

(i) $\det A \neq 0$ (A2.4a)

(ii) $\mathrm{Re}\, A$ be non-negative (eigenvalues ≥ 0). (A2.4b)

In particular, the case where $\det B = 0$ (a zero eigenvalue) seems not so well known. Clearly any non-zero eigenvalue of B must be positive. If all eigenvalues are non-zero (B positive), then B and C can be simultaneously diagonalised by an (in general) non-orthogonal real transformation with matrix Λ [5], giving

$$\begin{aligned} q^T A q &= X^T(E + \mathrm{i}\Gamma)X \\ &= \sum_{i=1}^{n}(1 + \mathrm{i}\gamma_j)X_j^2. \end{aligned} \tag{A2.5}$$

The resulting integral (A2.1) is

$$\begin{aligned} I(A) &= |\det\Lambda|\pi^{n/2}\left(\prod_{i=1}^{n}(1 + \mathrm{i}\gamma_i)\right)^{-1/2} \\ &= (\pi^n/\det A)^{1/2} \end{aligned} \tag{A2.6}$$

where $|\det \Lambda|$ is the Jacobian factor. If all eigenvalues are zero ($B=0$), the eigenvalues c_j of C determine the integral, which exists and is again given by (A2.6) iff no c_j vanishes ($\det A \neq 0$). In both cases the conditions (A2.4) obtain.

If B has n_0 zero eigenvalues ($0<n_0<n$), the original quadratic form can be transformed by some Λ' matrix to the form

$$q^T A q = [x, y]\begin{bmatrix} \mathrm{i}c_x & \mathrm{i}C'^T \\ \mathrm{i}C' & D \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} \qquad D \equiv E + \mathrm{i}c_y \tag{A2.7}$$

where x and y are vectors in zero and non-zero eigenvalue subspaces of B, respectively, c_x, c_y are corresponding diagonal submatrices of C and C' is real. In the y integrations, if done first, the finite displacement

$$y \to y' = y + \mathrm{i}D^{-1}C'x \tag{A2.8}$$

will not change the result. The effect of (A2.8) is to replace the matrix in equation (A2.7) by

$$A' = \begin{bmatrix} A_2 & 0 \\ 0 & D \end{bmatrix} \qquad A_2 = B_2 + \mathrm{i}C_2 \tag{A2.9}$$

with B_2 and C_2 real and

$$B_2 \equiv (D^{-1}C')^+ D^{-1}C' \tag{A2.10}$$

is non-negative.

Since the displacement (A2.8) corresponds to row and column operations on the determinant of the matrix in equation (A2.7), the determinant of A' has the same value. (Note that (A2.8), being complex, can produce a positive matrix B_2 although B has zero eigenvalues.)

The matrix A_2 can be treated in the same manner as was the original A, etc, until eventually a diagonal $n \times n$ matrix $A^{(f)}$ is reached which has either the form, $A_\alpha = E_n + \mathrm{i}\Gamma_n$, or the form A_β, comprised of diagonal submatrices $\mathrm{i}\Gamma_{n'}$ and $E_{n-n'} + \mathrm{i}\Gamma_{n-n'}$. The α form leads, as did (A2.5), to the value (A2.6) and the β form does likewise iff all the diagonal values in $\Gamma_{n'}$ are non-zero ($\det A \neq 0$).

Finally we remark on the convergence of integrals like (A2.1) when the q are also complex. Gaussian integrals in so-called holomorphic variables occur in functional integrals of field theory [6]. The standard result given is

$$\int \prod_{k=1}^{n} \left(\frac{\mathrm{d}z_k^* \, \mathrm{d}z_k}{2\pi \mathrm{i}}\right) \exp\left(-\sum_{i,j=1}^{n} z_i^* A_{ij} z_j\right) = \frac{1}{\det A} \tag{A2.11}$$

where $z_k = x_k + \mathrm{i}y_k$ and $z_k^* = x_k - \mathrm{i}y_k$ and

$$\int \frac{\mathrm{d}z^* \, \mathrm{d}z}{2\pi \mathrm{i}} = \int \frac{\mathrm{d}x \, \mathrm{d}y}{\pi}. \tag{A2.12}$$

The matrix A is in general not symmetric (see, e.g., equation (2.25) of reference [6]). The integral (A2.11) is equivalent to a $2n$-fold real integral (A2.1). The quadratic form in the real quantities x_k and y_k has the (symmetric) matrix

$$A' = \frac{1}{2}\begin{pmatrix} A_s & \mathrm{i}A_a \\ -\mathrm{i}A_a & A_s \end{pmatrix} \qquad (2n \times 2n) \tag{A2.13}$$

where $A_s = A + A^T$ and $A_a = A - A^T$. In terms of A the conditions (A2.4) for A' become

(i) $\det A \neq 0$

(ii) $A + A^{+}$ is non-negative. (A2.14)

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