Matsubara Summations & An Effective Electron-Phonon Action

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1 Matsubara Sums

Summations over Matsubara frequencies are often more easily evaluated as contour integrals in the complex domain.

This is done by introducing an auxiliary function, here denoted $g(z)$, that has simple poles at each Matsubara frequency ω_n; such that integration over a suitable contour returns the sum of interest as a sum of residues, as below.

$$\begin{aligned}\sum_n h(\omega_n) &= \frac{\xi}{2\pi i}\oint dz\ g(z)h(-iz) \\ &= \xi \sum_n \text{Res}\big[g(z)h(-iz)\big]\big|_{z=i\omega_n}\end{aligned}$$

Typical choices for $g(z)$ thus include the following (where the choice depends on whether the frequencies correspond to Fermions or Bosons):

$$g(z) = \begin{cases} \frac{\beta}{e^{\beta z}-1} & \text{(boson)} \\ \frac{\beta}{e^{\beta z}+1} & \text{(fermion)} \end{cases}$$

1.1 Evaluation of Pair Correlation Function

We now apply this formalism to the specific example of the *pair correlation function* $\chi^c_{n,\mathbf{q}}$, defined below.

$$\chi^c_{n,\mathbf{q}} = -\frac{k_B T}{V}\sum_{m,\mathbf{p}} G_0(\mathbf{p}, i\omega_m)G_0(-\mathbf{p}+\mathbf{q}, -i\omega_m + i\omega_n)$$

where

$$G_0(\mathbf{p}, i\omega_n) = \frac{1}{i\omega_m - \xi_\mathbf{p}}$$

is the relevant Green's function; and the convention here is that $i\omega_m = (2m+1)\pi/\beta$ are Fermionic Matsubara frequencies and $i\omega_n = 2n\pi/\beta$ are Bosonic Matsubara frequencies.

To garner a simpler form of the pair correlation function, we wish evaluate the sum over the Fermionic Matsubara frequencies. The means to evaluate this sum is made explicit by identifying $h(z)$, discussed in the previous section, to be $G_0(\mathbf{p}, z)G_0(-\mathbf{p}+\mathbf{q}, -z+i\omega_n)$ in this case. Expanding the Green's functions, it's then clear that $h(z)$ has (simple) poles for arguments $z = \xi_\mathbf{p}$ and $z = i\omega_n - \xi_{-\mathbf{p}+\mathbf{q}}$.

Then, choosing $g(z) = \beta/(e^{\beta z}+1)$, we may simply sum over all the residues of the product $g(z)h(-iz)$, as specified in the introduction. This yields the following equality:

$$\chi^c_{n,\mathbf{q}} = -\frac{1}{V}\sum_\mathbf{p} \frac{-n(\xi_p) + n(-\xi_{p-q} + i\omega_n)}{i\omega_n - \xi_p - \xi_{-p+q}}$$

where $n(x)$ is the Fermi-Dirac distribution function, defined as below.

$$n(x) = \frac{1}{e^{\beta x}+1}$$

With the expression of $n(x)$ in sight, it's easy to verify then that $n(x+2\pi i n) = n(x)$ and $n(-x) = 1 - n(x)$, allowing us to simplify further, so that we have the final expression for the pair correlation function given below.

$$\chi^c_{n,\mathbf{q}} = -\frac{1}{V}\sum_\mathbf{p} \frac{1 - n(\xi_p) - n(\xi_{-p+q})}{i\omega_n - \xi_p - \xi_{-p+q}}$$

1.2 Evaluation of Density Correlation Function

Now we apply this formalism to the *density correlation function* $\chi^d_{n,\mathbf{q}}$, defined below.

$$\chi^d_{n,\mathbf{q}} = -\frac{k_B T}{V}\sum_{m,\mathbf{p}} G_0(\mathbf{p}, i\omega_m)G_0(\mathbf{p}+\mathbf{q}, i\omega_m + i\omega_n)$$

Similar to the previous case of the pair correlation function, we now identify $h(z) = G_0(\mathbf{p}, z)G_0(\mathbf{p}+\mathbf{q}, z+i\omega_n)$ which has (simple) poles at $z = \xi_\mathbf{p}$ and $z = -i\omega_n + \xi_{\mathbf{p}+\mathbf{q}}$. Again summing over the residues of these poles, we arrive at a form for our considered correlation function:

$$\begin{aligned}\chi^d_{n,\mathbf{q}} &= \frac{1}{V}\sum_\mathbf{p} \frac{-n(\xi_p) + n(\xi_{-p-q} - i\omega_n)}{i\omega_n - \xi_p + \xi_{p+q}} \\ &= \frac{1}{V}\sum_\mathbf{p} \frac{-n(\xi_p) + n(\xi_{-p-q})}{i\omega_n - \xi_p + \xi_{p+q}}\end{aligned}$$

where we've again used $n(x+2\pi i n) = n(x)$.

2 Electron-Phonon Coupling

The total action of a material in which electrons and phonons exist and interact can be decomposed into a sum of three terms, corresponding to the electron free field, phonon free field, and interaction term between the two; as below:

$$S[\bar{\phi}, \phi, \bar{\psi}, \psi] = S_{el}[\bar{\psi}, \psi] + S_{ph}[\bar{\phi}, \phi] + S_{el-ph}[\bar{\phi}, \phi, \bar{\psi}, \psi]$$

where $\bar{\psi}, \psi$ are (independent) Grassman fields corresponding to the electrons and $\bar{\phi}, \phi$ are complex fields corresponding to the phonons. The phonon and interaction terms then have the following forms:

$$S_{ph}[\bar{\phi}, \phi] = \sum_{q,j} \bar{\phi}_{qj}(-i\omega_n + \omega_q)\phi_{qj}$$

$$S_{el-ph}[\bar{\psi}, \psi, \bar{\phi}, \phi] = \gamma \sum_{q,j} \frac{iq_j}{\sqrt{2m\omega_q}}(\bar{\phi}_{-qj} + \phi_{qj})\rho_q$$

where we've used the shorthand notation $q = (\mathbf{q}, \omega_n)$ and summation over n is implied.

Now, to obtain an effective action, we can exponentiate the action, integrate over the fields we'd like to ignore (here the complex fields $\bar{\phi}, \phi$), and then take the natural logarithm of the result, as below.

$$S_{\text{ef}}[\bar{\psi}, \psi] = -\ln\Big(\int D[\bar{\phi}, \phi]\ e^{-S[\bar{\phi}, \phi, \bar{\psi}, \psi]}\Big)$$
$$= S_{el}[\bar{\psi}, \psi] - \ln\Big(\int D[\bar{\phi}, \phi]\ e^{-(S_p[\bar{\phi}, \phi] + S_{e-p}[\bar{\phi}, \phi, \bar{\psi}, \psi])}\Big)$$

where the electron term of the action is unaffected due to it's independence of $\bar{\phi}, \phi$. Let us now consider the integral over the remaining exponential term:

$$\int D[\bar{\phi}, \phi]\, e^{-\sum_{q,j}\left(\bar{\phi}_{qj}(-i\omega_n + \omega_q)\phi_{qj} + \gamma\frac{iq_j}{\sqrt{2m\omega_q}}(\bar{\phi}_{-qj} + \phi_{qj})\rho_q\right)}$$

The argument of the exponential then may be rewritten such that it resembles a Gaussian integral, as below:

$$\sum_{q,j}\Big(\bar{\phi}_{qj}(-i\omega_n + \omega_q)\phi_{qj} + \gamma\frac{iq_j}{\sqrt{2m\omega_q}}(\bar{\phi}_{-qj} + \phi_{qj})\rho_q\Big)$$
$$= \frac{1}{2}\sum_{q,j}\Bigg(\begin{bmatrix}\bar{\phi}_{qj} & \phi_{qj}\end{bmatrix}\begin{bmatrix}-i\omega_n + \omega_q & 0 \\ 0 & -i\omega_n + \omega_q\end{bmatrix}\begin{bmatrix}\bar{\phi}_{qj} \\ \phi_{qj}\end{bmatrix}$$
$$+ \gamma\frac{iq_j}{\sqrt{2m\omega_q}}\Big(\begin{bmatrix}\bar{\phi}_{-qj} & \phi_{qj}\end{bmatrix}\begin{bmatrix}1 \\ 1\end{bmatrix} + \begin{bmatrix}1 & 1\end{bmatrix}\begin{bmatrix}\bar{\phi}_{-qj} \\ \phi_{qj}\end{bmatrix}\Big)\rho_q\Bigg)$$

Now making the identifications below,

$$A = \begin{bmatrix}-i\omega_n + \omega_q & 0 \\ 0 & -i\omega_n + \omega_q\end{bmatrix}$$

$$b = \begin{bmatrix}1 \\ 1\end{bmatrix}$$

we may apply the general Gaussian integral formula:

$$\int D(x)\exp\Big(-\frac{1}{2}v^T A v + b\cdot x\Big)$$
$$= \sqrt{\frac{(2\pi)^2}{|A|}}\exp\Big(\frac{1}{2}b^T A^{-1} b\Big)$$

After applying the logarithm, we then arrive at the desired form for the effective action of the electrons below.

$$S_{eff}[\bar{\psi}, \psi] = S_{el}[\bar{\psi}, \psi] - \frac{\gamma}{2m}\sum_q \frac{q^2}{\omega_n^2 + \omega_q^2}\rho_q\rho_{-q}$$