atoms

MDPI

Article

Supplemental Materials: Response Functions

Patrick Kelly and Ettore Vitali *

Department of Physics, California State University Fresno, Fresno, CA 93740, USA; ptfk121493@mail.fresnostate.edu
* Correspondence: evitali@csufresno.edu

check for updates

Citation: Kelly, P.; Vitali, E. Supplemental Materials: Response Functions. *Atoms* **2021**, *9*, 88. https://doi.org/10.3390/atoms9040088

Academic Editor: Nicola Piovella

Received: 13 September 2021
Accepted: 23 October 2021
Published: 26 October 2021

1. BCS Response Functions

Here we give the explicit expressions for all the BCS response functions (the matrix elements in equation (12) in the main text) used in our study. Below, $u(\mathbf{k})$ and $v(\mathbf{k})$ are the coefficients of the BCS wave function:

$$|\Psi_{BCS}\rangle = \prod_{\mathbf{k}}\left(u(\mathbf{k}) + v(\mathbf{k})\hat{c}^{\dagger}_{\mathbf{k},\uparrow}\hat{c}^{\dagger}_{-\mathbf{k},\downarrow}\right)|0\rangle \tag{S1}$$

and are given by:

$$u^2(\mathbf{k}) = \frac{1}{2}\left(1 + \frac{\xi(\mathbf{k})}{\sqrt{\xi(\mathbf{k})^2 + \Delta^2_{BCS}}}\right), \quad v^2(\mathbf{k}) = \frac{1}{2}\left(1 - \frac{\xi(\mathbf{k})}{\sqrt{\xi(\mathbf{k})^2 + \Delta^2_{BCS}}}\right) \tag{S2}$$

In the above:

$$\xi(\mathbf{k}) = \varepsilon(\mathbf{k}) - \mu_{BCS} \tag{S3}$$

We also define:

$$E(\mathbf{k}) = \sqrt{\xi(\mathbf{k})^2 + \Delta^2_{BCS}} \tag{S4}$$

The GRPA calculation needs to be preceded by a standard BCS calculation to find μ_{BCS} and Δ_{BCS}.

$$\chi^0_{11}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{v^\star(\mathbf{k})u(\mathbf{k}-\mathbf{K})v(\mathbf{k})u^\star(\mathbf{k}-\mathbf{K})}{\omega + E(\mathbf{k}-\mathbf{K}) + E(-\mathbf{k}) + i0^+} - \frac{u(\mathbf{k}+\mathbf{K})v^\star(\mathbf{k})u^\star(\mathbf{k}+\mathbf{K})v(\mathbf{k})}{\omega - E(\mathbf{k}+\mathbf{K}) - E(-\mathbf{k}) + i0^+}\right) \tag{S5}$$

$$\chi^0_{12}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{v(\mathbf{k}-\mathbf{K})u^\star(\mathbf{k})v(\mathbf{k})u^\star(\mathbf{k}-\mathbf{K})}{\omega + E(\mathbf{k}-\mathbf{K}) + E(-\mathbf{k}) + i0^+} - \frac{u(\mathbf{k}+\mathbf{K})v^\star(\mathbf{k})u(\mathbf{k})v^\star(\mathbf{k}+\mathbf{K})}{\omega - E(\mathbf{k}+\mathbf{K}) - E(-\mathbf{k}) + i0^+}\right) \tag{S6}$$

$$\chi^0_{13}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{u^\star(\mathbf{k})u(\mathbf{k}-\mathbf{K})v(\mathbf{k})u^\star(\mathbf{k}-\mathbf{K})}{\omega + E(\mathbf{k}-\mathbf{K}) + E(-\mathbf{k}) + i0^+} + \frac{u(\mathbf{k}+\mathbf{K})v^\star(\mathbf{k})v^\star(\mathbf{k}+\mathbf{K})v(\mathbf{k})}{\omega - E(\mathbf{k}+\mathbf{K}) - E(-\mathbf{k}) + i0^+}\right) \tag{S7}$$

$$\chi^0_{14}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{-v^\star(\mathbf{k})v(\mathbf{k}-\mathbf{K})v(\mathbf{k})u^\star(\mathbf{k}-\mathbf{K})}{\omega + E(\mathbf{k}-\mathbf{K}) + E(-\mathbf{k}) + i0^+} - \frac{u(\mathbf{k}+\mathbf{K})v^\star(\mathbf{k})u^\star(\mathbf{k})u(\mathbf{k}+\mathbf{K})}{\omega - E(\mathbf{k}+\mathbf{K}) - E(-\mathbf{k}) + i0^+}\right) \tag{S8}$$

$$\chi^0_{21}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{v^\star(\mathbf{k})u(\mathbf{k}-\mathbf{K})v^\star(\mathbf{k}-\mathbf{K})u(\mathbf{k})}{\omega+E(\mathbf{k}-\mathbf{K})+E(-\mathbf{k})+i0^+} - \frac{u^\star(\mathbf{k})v(\mathbf{k}+\mathbf{K})u^\star(\mathbf{k}+\mathbf{K})v(\mathbf{k})}{\omega-E(\mathbf{k}+\mathbf{K})-E(-\mathbf{k})+i0^+}\right) \tag{S9}$$

$$\chi^0_{22}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{v(\mathbf{k}-\mathbf{K})u^\star(\mathbf{k})v^\star(\mathbf{k}-\mathbf{K})u(\mathbf{k})}{\omega+E(\mathbf{k}-\mathbf{K})+E(-\mathbf{k})+i0^+} - \frac{u^\star(\mathbf{k})v(\mathbf{k}+\mathbf{K})u(\mathbf{k})v^\star(\mathbf{k}+\mathbf{K})}{\omega-E(\mathbf{k}+\mathbf{K})-E(-\mathbf{k})+i0^+}\right) \tag{S10}$$

$$\chi^0_{23}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{u^\star(\mathbf{k})u(\mathbf{k}-\mathbf{K})v^\star(\mathbf{k}-\mathbf{K})u(\mathbf{k})}{\omega+E(\mathbf{k}-\mathbf{K})+E(-\mathbf{k})+i0^+} + \frac{u^\star(\mathbf{k})v(\mathbf{k}+\mathbf{K})v^\star(\mathbf{k}+\mathbf{K})v(\mathbf{k})}{\omega-E(\mathbf{k}+\mathbf{K})-E(-\mathbf{k})+i0^+}\right) \tag{S11}$$

$$\chi^0_{24}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{-v^\star(\mathbf{k})v(\mathbf{k}-\mathbf{K})v^\star(\mathbf{k}-\mathbf{K})u(\mathbf{k})}{\omega+E(\mathbf{k}-\mathbf{K})+E(-\mathbf{k})+i0^+} - \frac{u^\star(\mathbf{k})v(\mathbf{k}+\mathbf{K})u^\star(\mathbf{k})u(\mathbf{k}+\mathbf{K})}{\omega-E(\mathbf{k}+\mathbf{K})-E(-\mathbf{k})+i0^+}\right) \tag{S12}$$

$$\chi^0_{31}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{v^\star(\mathbf{k})u(\mathbf{k}-\mathbf{K})u(\mathbf{k})u^\star(\mathbf{k}-\mathbf{K})}{\omega+E(\mathbf{k}-\mathbf{K})+E(-\mathbf{k})+i0^+} + \frac{v(\mathbf{k}+\mathbf{K})v^\star(\mathbf{k})u^\star(\mathbf{k}+\mathbf{K})v(\mathbf{k})}{\omega-E(\mathbf{k}+\mathbf{K})-E(-\mathbf{k})+i0^+}\right) \tag{S13}$$

$$\chi^0_{32}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{v(\mathbf{k}-\mathbf{K})u^\star(\mathbf{k})u(\mathbf{k})u^\star(\mathbf{k}-\mathbf{K})}{\omega+E(\mathbf{k}-\mathbf{K})+E(-\mathbf{k})+i0^+} + \frac{v(\mathbf{k}+\mathbf{K})v^\star(\mathbf{k})u(\mathbf{k})v^\star(\mathbf{k}+\mathbf{K})}{\omega-E(\mathbf{k}+\mathbf{K})-E(-\mathbf{k})+i0^+}\right) \tag{S14}$$

$$\chi^0_{33}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{u^\star(\mathbf{k})u(\mathbf{k}-\mathbf{K})u(\mathbf{k})u^\star(\mathbf{k}-\mathbf{K})}{\omega+E(\mathbf{k}-\mathbf{K})+E(-\mathbf{k})+i0^+} - \frac{v(\mathbf{k}+\mathbf{K})v^\star(\mathbf{k})v^\star(\mathbf{k}+\mathbf{K})v(\mathbf{k})}{\omega-E(\mathbf{k}+\mathbf{K})-E(-\mathbf{k})+i0^+}\right) \tag{S15}$$

$$\chi^0_{34}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{-v^\star(\mathbf{k})v(\mathbf{k}-\mathbf{K})u(\mathbf{k})u^\star(\mathbf{k}-\mathbf{K})}{\omega+E(\mathbf{k}-\mathbf{K})+E(-\mathbf{k})+i0^+} + \frac{v(\mathbf{k}+\mathbf{K})v^\star(\mathbf{k})u^\star(\mathbf{k})u(\mathbf{k}+\mathbf{K})}{\omega-E(\mathbf{k}+\mathbf{K})-E(-\mathbf{k})+i0^+}\right) \tag{S16}$$

$$\chi^0_{41}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{-v^\star(\mathbf{k})u(\mathbf{k}-\mathbf{K})v(\mathbf{k})v^\star(\mathbf{k}-\mathbf{K})}{\omega+E(\mathbf{k}-\mathbf{K})+E(-\mathbf{k})+i0^+} - \frac{u(\mathbf{k})u^\star(\mathbf{k}+\mathbf{K})u^\star(\mathbf{k}+\mathbf{K})v(\mathbf{k})}{\omega-E(\mathbf{k}+\mathbf{K})-E(-\mathbf{k})+i0^+}\right) \tag{S17}$$

$$\chi^0_{42}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{-v(\mathbf{k}-\mathbf{K})u^\star(\mathbf{k})v(\mathbf{k})v^\star(\mathbf{k}-\mathbf{K})}{\omega+E(\mathbf{k}-\mathbf{K})+E(-\mathbf{k})+i0^+} - \frac{u(\mathbf{k})u^\star(\mathbf{k}+\mathbf{K})u(\mathbf{k})v^\star(\mathbf{k}+\mathbf{K})}{\omega-E(\mathbf{k}+\mathbf{K})-E(-\mathbf{k})+i0^+}\right) \tag{S18}$$

$$\chi^0_{43}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{-u^\star(\mathbf{k})u(\mathbf{k}-\mathbf{K})v(\mathbf{k})v^\star(\mathbf{k}-\mathbf{K})}{\omega+E(\mathbf{k}-\mathbf{K})+E(-\mathbf{k})+i0^+} + \frac{u(\mathbf{k})u^\star(\mathbf{k}+\mathbf{K})v^\star(\mathbf{k}+\mathbf{K})v(\mathbf{k})}{\omega-E(\mathbf{k}+\mathbf{K})-E(-\mathbf{k})+i0^+}\right) \tag{S19}$$

$$\chi^0_{44}(\mathbf{K},\omega) = \frac{1}{V}\sum_{\mathbf{k}}\left(\frac{v^\star(\mathbf{k})v(\mathbf{k}-\mathbf{K})v(\mathbf{k})v^\star(\mathbf{k}-\mathbf{K})}{\omega+E(\mathbf{k}-\mathbf{K})+E(-\mathbf{k})+i0^+} - \frac{u(\mathbf{k})u^\star(\mathbf{k}+\mathbf{K})u^\star(\mathbf{k})u(\mathbf{k}+\mathbf{K})}{\omega-E(\mathbf{k}+\mathbf{K})-E(-\mathbf{k})+i0^+}\right) \tag{S20}$$

If we assume that $u, v \in \mathbb{R}$, then we have the following relations between the components:

$$\begin{aligned} &\chi^0_{12} = \chi^0_{21} = -\chi^0_{34} = -\chi^0_{43} \\ &\chi^0_{13} = \chi^0_{31} \\ &\chi^0_{14} = \chi^0_{41} \\ &\chi^0_{23} = \chi^0_{32} \\ &\chi^0_{24} = \chi^0_{42} \end{aligned} \tag{S21}$$