Two-Fermion Correlations in the Lieb-Lattice

July 7, 2025

1 The Model

The Lieb lattice is a square lattice with a three atom basis [1, 2]. The a atoms are located at the lattice sites and the b and c atoms, respectively, are positioned at the mid-points between closest neighboring lattice sites in the x and y directions, as depicted in Fig.(1). The Hamiltonian is expressed as

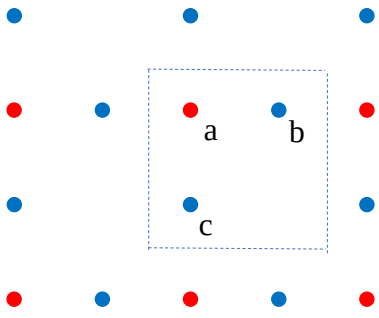

Figure 1: A sketch of the Lieb lattice which contains a sub-lattice of four-fold coordinated a sites and a sub-lattice of the two-fold coordinates b and c sites. The unit cell is enclosed by the dotted lines.

$$\hat{H} \;=\; \hat{H}_0 \;+\; \hat{H}_I \tag{1}$$

where $\hat{H}_0$ is the Hamiltonian for the non-interacting electrons and $\hat{H}_I$ represents the electron-electron interactions. The non-interacting Hamiltonian $\hat{H}_0$ is given by

$$\begin{aligned}\hat{H}_0 \;=\; & \sum_{\underline{R},\sigma} \frac{t}{2} \left[\left(a^{\dagger}_{\underline{R},\sigma}\, b_{\underline{R},\sigma} \;+\; b^{\dagger}_{\underline{R},\sigma}\, a_{\underline{R},\sigma} \right) \;+\; \left(a^{\dagger}_{\underline{R},\sigma}\, c_{\underline{R},\sigma} \;+\; c^{\dagger}_{\underline{R},\sigma}\, a_{\underline{R},\sigma} \right) \right] \\ & + \sum_{\underline{R},\sigma} \frac{t}{2} \left[\left(b^{\dagger}_{\underline{R},\sigma}\, a_{\underline{R}+\delta_x,\sigma} \;+\; a^{\dagger}_{\underline{R}+\delta_x,\sigma}\, b_{\underline{R},\sigma} \right) \;+\; \left(c^{\dagger}_{\underline{R},\sigma}\, a_{\underline{R}+\delta_y,\sigma} \;+\; a^{\dagger}_{\underline{R}+\delta_y,\sigma}\, c_{\underline{R},\sigma} \right) \right]\end{aligned}$$

(2)

where the sum over $\underline{R}$ is a sum over the lattice vectors and $\delta_x = \frac{a}{2}\hat{e}_x$ and $\delta_y = \frac{a}{2}\hat{e}_y$ are displacements by half a primitive lattice vector, and the operators $a^\dagger_{\underline{R},\sigma}$ and $a_{\underline{R},\sigma}$, respectively create and annihilate an electron on atom a with spin σ on the a site of the $\underline{R}$ unit cell. The interaction Hamiltonian is expressed as

$$\hat{H}_I \;=\; \frac{U}{2}\sum_{\underline{R},\alpha,\sigma}\left[\;\alpha^\dagger_{\underline{R},\sigma}\;\alpha^\dagger_{\underline{R},\overline{\sigma}}\;\alpha_{\underline{R},\overline{\sigma}}\;\alpha_{\underline{R},\sigma}\;\right] \tag{3}$$

where the sum over α runs over the three atomic basis sites $\alpha = a, b$ or c. The interaction represents highly screened local interactions between the electrons with opposite spins which are located on the same atomic site. In the Bloch representation, the non-interacting Hamiltonian takes the form

$$\hat{H}_0 \;=\; \sum_{\underline{k},\sigma} t\left[\;\cos\frac{k_x a}{2}\;(\;a^\dagger_{\underline{k},\sigma}\;b_{\underline{k},\sigma}\;+\;b^\dagger_{\underline{k},\sigma}\;a_{\underline{k},\sigma}\;)\;+\;\cos\frac{k_y a}{2}\;(\;a^\dagger_{\underline{k},\sigma}\;c_{\underline{k},\sigma}\;+\;c^\dagger_{\underline{k},\sigma}\;a_{\underline{k},\sigma}\;)\;\right] \tag{4}$$

The high symmetry points of the Brillouin zone are identified in Fig. (2). The

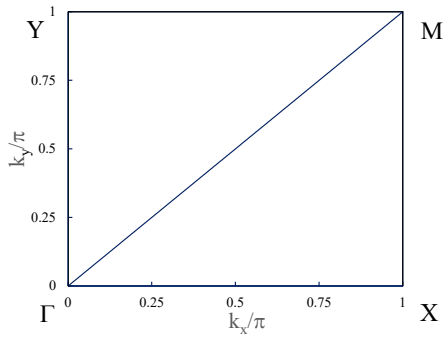

Figure 2: The high-symmetry lines and high symmetry points of the Lieb Lattice Brillouin zone.

transformed interaction Hamiltonian has the form of a sum of three separable interactions

$$\hat{H}_I \;=\; \frac{U}{2\;N}\sum_{\alpha,\underline{k},\underline{k}',\underline{q},\sigma}\left[\;\alpha^\dagger_{\underline{k},\sigma}\;\alpha^\dagger_{\underline{k}',\overline{\sigma}}\;\alpha_{\underline{k}'-\underline{q},\overline{\sigma}}\;\alpha_{\underline{k}+\underline{q},\sigma}\right] \tag{5}$$

where $\alpha \;\in\; \{a, b, c\}$.

2 One-Electron Green's Functions

The time-ordered one-electron Green's functions are defined as

$$G^{\alpha,\beta}_{k,\sigma;k',\sigma'}(t,t') \;=\; -\,\frac{i}{\hbar}\,\langle\,|\,\hat{T}\;\alpha_{k,\sigma}(t)\;,\;\beta^{\dagger}_{k',\sigma'}(t')\,|\,\rangle \tag{6}$$

where $\hat{T}$ is Wick's time-ordering operator and the vacuum state is denoted by $|\,\rangle$. The equations of motion for the one-electron Green's function are

$$\begin{aligned} i\;\hbar\;\frac{\partial}{\partial t}G^{\alpha,\beta}_{k,\sigma;k',\sigma'}(t,t') \;&=\; \delta(t-t')\;\langle\,|\,\{\;\alpha_{k,\sigma}(t)\;,\;\beta^{\dagger}_{k',\sigma'}(t')\;\}_{+}\,|\,\rangle \\ &\quad -\,\frac{i}{\hbar}\;\langle\,|\,\hat{T}\;[\;\alpha_{k,\sigma}(t)\;,H(t)\;]\;,\;\beta^{\dagger}_{k',\sigma'}(t')\,|\,\rangle \end{aligned} \tag{7}$$

The equations of motion reduce to:

$$\begin{aligned} i\;\hbar\;\frac{\partial}{\partial t}G^{a,\beta}_{k,\sigma;k',\sigma'}(t,t') \;&=\; \delta(t-t')\;\delta^{a,\beta}\;\delta_{k,k'}\;\delta_{\sigma,\sigma'} \\ &\quad +\;t\;\cos\frac{k_x}{2}\;G^{b,\beta}_{k,\sigma;k',\sigma'}(t,t')\;+\;t\;\cos\frac{k_y}{2}\;G^{c,\beta}_{k,\sigma;k',\sigma'}(t,t') \\ i\;\hbar\;\frac{\partial}{\partial t}G^{b,\beta}_{k,\sigma;k',\sigma'}(t,t') \;&=\; \delta(t-t')\;\delta^{b,\beta}\;\delta_{k,k'}\;\delta_{\sigma,\sigma'}\;+\;t\;\cos\frac{k_x}{2}\;G^{a,\beta}_{k,\sigma;k',\sigma'}(t,t') \\ i\;\hbar\;\frac{\partial}{\partial t}G^{c,\beta}_{k,\sigma;k',\sigma'}(t,t') \;&=\; \delta(t-t')\;\delta^{c,\beta}\;\delta_{k,k'}\;\delta_{\sigma,\sigma'}\;+\;t\;\cos\frac{k_y}{2}\;G^{a,\beta}_{k,\sigma;k',\sigma'}(t,t') \end{aligned} \tag{8}$$

The interaction term vanishes, since it is normal ordered and its commutators are evaluated in the vacuum state. Fourier transforming the equations of motion yields a closed set of linear coupled algebraic equations

$$\begin{aligned} \hbar\;\omega\;G^{a,\beta}_{k,\sigma;k',\sigma'}(\omega) \;&=\; \delta^{a,\beta}\;\delta_{k,k'}\;\delta_{\sigma,\sigma'} \\ &\quad +\;t\;\cos\frac{k_x}{2}\;G^{b,\beta}_{k,\sigma;k',\sigma'}(\omega)\;+\;t\;\cos\frac{k_y}{2}\;G^{c,\beta}_{k,\sigma;k',\sigma'}(\omega) \\ \hbar\;\omega\;G^{b,\beta}_{k,\sigma;k',\sigma'}(\omega) \;&=\; \delta^{b,\beta}\;\delta_{k,k'}\;\delta_{\sigma,\sigma'}\;+\;t\;\cos\frac{k_x}{2}\;G^{a,\beta}_{k,\sigma;k',\sigma'}(\omega) \\ \hbar\;\omega\;G^{c,\beta}_{k,\sigma;k',\sigma'}(\omega) \;&=\; \delta^{c,\beta}\;\delta_{k,k'}\;\delta_{\sigma,\sigma'}\;+\;t\;\cos\frac{k_y}{2}\;G^{a,\beta}_{k,\sigma;k',\sigma'}(\omega) \end{aligned} \tag{9}$$

in order to guarantee convergence when $t-t' \rightarrow\;\infty$, ω must be evaluated at a complex frequency $\omega + i\eta$ where η is a positive infinitesimal constant. These equations can be solved to give

$$\begin{pmatrix} G^{a,\beta}_{k,\sigma;k',\sigma'}(\omega) \\ G^{b,\beta}_{k,\sigma;k',\sigma'}(\omega) \\ G^{c,\beta}_{k,\sigma;k',\sigma'}(\omega) \end{pmatrix} \;=\; \frac{\delta_{k,k'}\;\delta_{\sigma,\sigma'}}{\hbar\omega\;\left[\hbar^2\omega^2\;-t^2(\cos^2\frac{k_x}{2}+\cos^2\frac{k_y}{2})\right]}\;\times$$

$$\left(\begin{array}{ccc} \hbar^2\omega^2 & \hbar\omega\ t\cos\frac{k_x}{2} & \hbar\omega\ t\cos\frac{k_y}{2} \\ \hbar\omega\ t\cos\frac{k_x}{2} & \hbar^2\omega^2 - t^2\cos^2\frac{k_y}{2} & t^2\cos\frac{k_x}{2}\cos\frac{k_y}{2} \\ \hbar\omega\ t\cos\frac{k_y}{2} & t^2\cos\frac{k_x}{2}\cos\frac{k_y}{2} & \hbar^2\omega^2 - t^2\cos^2\frac{k_x}{2} \end{array} \right) \left(\begin{array}{c} \delta^{a,\beta} \\ \delta^{b,\beta} \\ \delta^{c,\beta} \end{array} \right) \tag{10}$$

The dispersion relations are given by the poles of the Green's function and are found at $\hbar\omega = \epsilon_m(k)$, where

$$\begin{aligned} \epsilon_0(k) &= 0 \\ \epsilon_\pm(k) &= \pm\,|t|\,\sqrt{\cos^2\frac{k_x}{2} + \cos^2\frac{k_y}{2}} \end{aligned} \tag{11}$$

The single-electron Green's functions can be reduced to the form

$$G^{\alpha,\beta}_{k,\sigma;k',\sigma'}(\omega) = \delta_{\sigma,\sigma'}\delta_{k,k'}\ \sum_m\ \frac{A^\alpha_m(k)^*\ A^\beta_m(k)}{\hbar\omega - \epsilon_m(k)} \tag{12}$$

where the site-diagonal spectral weights are given by

$$\begin{aligned} |\ A^a_\pm(k)\ |^2 &= \frac{1}{2} \\ |\ A^b_\pm(k)\ |^2 &= \frac{1}{2}\ \frac{\cos^2\frac{k_x}{2}}{\cos^2\frac{k_x}{2} + \cos^2\frac{k_y}{2}} \\ |\ A^c_\pm(k)\ |^2 &= \frac{1}{2}\ \frac{\cos^2\frac{k_y}{2}}{\cos^2\frac{k_x}{2} + \cos^2\frac{k_y}{2}} \\ |\ A^b_0(k)\ |^2 &= \frac{\cos^2\frac{k_y}{2}}{\cos^2\frac{k_x}{2} + \cos^2\frac{k_y}{2}} \\ |\ A^c_0(k)\ |^2 &= \frac{\cos^2\frac{k_x}{2}}{\cos^2\frac{k_x}{2} + \cos^2\frac{k_y}{2}} \end{aligned} \tag{13}$$

and the site off-diagonal spectral weights are

$$\begin{aligned} A^a_\pm(k)\ A^b_\pm(k) &= \mp\,\frac{1}{2}\ \frac{\cos\frac{k_x}{2}}{\sqrt{\cos^2\frac{k_x}{2} + \cos^2\frac{k_y}{2}}} \\ A^a_\pm(k)\ A^c_\pm(k) &= \mp\,\frac{1}{2}\ \frac{\cos\frac{k_y}{2}}{\sqrt{\cos^2\frac{k_x}{2} + \cos^2\frac{k_y}{2}}} \\ A^b_\pm(k)\ A^c_\pm(k) &= \frac{1}{2}\ \frac{\cos\frac{k_x}{2}\cos\frac{k_y}{2}}{\cos^2\frac{k_x}{2} + \cos^2\frac{k_y}{2}} \\ A^b_0(k)\ A^c_0(k) &= -\ \frac{\cos\frac{k_x}{2}\cos\frac{k_y}{2}}{\cos^2\frac{k_x}{2} + \cos^2\frac{k_y}{2}} \end{aligned} \tag{14}$$

where we are mindful that t is negative. Hence, the one-electron Hamiltonian is diagonalized by the one-electron creation, $\gamma^{\dagger}_{m,\underline{k},\sigma}$ and annihilation operators, $\gamma_{m,\underline{k},\sigma}$, and is given by

$$\hat{H}_0 \quad = \quad \sum_{m,\underline{k},\sigma} \epsilon_m(\underline{k})\ \gamma^{\dagger}_{m,\underline{k},\sigma}\ \gamma_{m,\underline{k},\sigma} \tag{15}$$

where the diagonal band operators are related to the operators in the site representation via

$$\gamma^{\dagger}_{m,\underline{k},\sigma} \quad = \quad \sum_{\alpha} A^{\alpha}_{m}(\underline{k})\ \alpha^{\dagger}_{\underline{k},\sigma} \tag{16}$$

The dispersion relations for the one-electron excitations along the high-symmetry lines of the Brillouin zone, are shown in Fig.(3). Since the chiral operator anti-

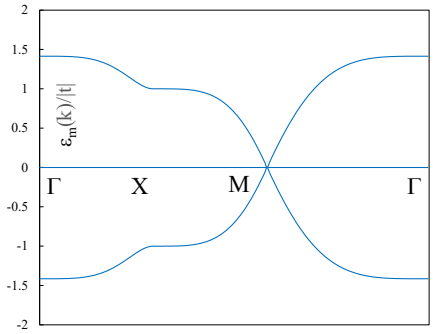

Figure 3: The three dispersion relations for the one-electron excitations of the Hubbard-Lieb Lattice, along the high-symmetry lines of the Brillouin zone. Note the three-fold degeneracy of the bands at the M point.

commutes with the Bloch Hamiltonian, the energy eigenvalues of the Bloch states are anti-symmetric under $\epsilon_k \ \rightarrow -\epsilon_k$, consequently the flat band exists at $\epsilon_k = 0$ due to the odd number of sites per unit cell. It should be noted that the dispersive bands becomes degenerate with the non-dispersive band at the M point of the Brillouin zone, as seen in Fig. (3). Also note that the spectral weights of the b and c states are equal along the high-symmetry line ΓM for which $k_x = k_y$, and that the discontinuity at M is a consequence of the "Hairy Ball" Theorem [3] since the Green's function is performing a mapping of states described on a toroidal Brilloiun zone onto a three-dimensional Hilbert space.

3 The Interaction Hamiltonian

The interaction is assumed to be a screened Coulomb interaction of strength U, which when expressed in terms of the band-diagonal electron creation and

annihilation operators has the form of the sum of three separable terms

$$\hat{H}_{int} = \frac{U}{N} \sum_{\underline{q},\alpha} \Bigg[\sum_{\underline{k}',m,n} A^{\alpha}_{m}\left(\frac{\underline{q}}{2}+\underline{k}'\right) A^{\alpha}_{n}\left(\frac{\underline{q}}{2}-\underline{k}'\right) \gamma^{\dagger}_{m,\frac{\underline{q}}{2}+\underline{k}',\uparrow} \gamma^{\dagger}_{n,\frac{\underline{q}}{2}-\underline{k}',\downarrow} \times \sum_{\underline{k},s,t} A^{\alpha}_{s}\left(\frac{\underline{q}}{2}-\underline{k}\right) A^{\alpha}_{t}\left(\frac{\underline{q}}{2}+\underline{k}\right) \gamma_{s,\frac{\underline{q}}{2}-\underline{k},\downarrow} \gamma_{t,\frac{\underline{q}}{2}+\underline{k},\uparrow} \Bigg] \tag{17}$$

4 The Two-Electron's Green's Function

We define the two-electron Green's Function in terms of the diagonal one-electron basis operators as a time-ordered, two-point correlation function

$$G_{m,n,s,t}(q;k,t;k',t') = -\frac{i}{\hbar} \langle \mid \hat{T}\ \gamma_{m,\frac{q}{2}+k,\sigma}(t)\ \gamma_{n,\frac{q}{2}-k,\overline{\sigma}}(t)\ \gamma^{\dagger}_{s,\frac{q}{2}-k',\overline{\sigma}}(t')\ \gamma^{\dagger}_{t,\frac{q}{2}+k',\sigma}(t') \mid \rangle \tag{18}$$

where $\underline{q}$ represents the center of mass momentum. The two-electron Green's functions satisfy the equations of motion

$$\begin{aligned} &\left(i\,\hbar\,\frac{\partial}{\partial t} - \epsilon_m\left(\frac{q}{2}+k\right) - \epsilon_n\left(\frac{q}{2}-k\right) \right) G_{m,n,s,t}(q;k,t;k',t') \\ &= \delta(t-t')\ \langle \mid \{\ \gamma_{m,\frac{q}{2}+k,\sigma}(t)\ \gamma_{n,\frac{q}{2}-k,\overline{\sigma}}(t)\ ,\ \gamma^{\dagger}_{s,\frac{q}{2}-k',\overline{\sigma}}(t')\ \gamma^{\dagger}_{t,\frac{q}{2}+k',\sigma}(t')\} \mid \rangle \\ &\quad + \langle \mid \hat{T}\ \Big[\ \gamma_{m,\frac{q}{2}+k,\sigma}(t)\ \gamma_{n,\frac{q}{2}-k,\overline{\sigma}}(t)\ ,\ \hat{H}_{int}(t')\ \Big]\ \gamma^{\dagger}_{s,\frac{q}{2}-k',\overline{\sigma}}(t')\ \gamma^{\dagger}_{t,\frac{q}{2}+k',\sigma}(t') \mid \rangle \end{aligned} \tag{19}$$

Putting the anticommutator into normal ordered form and evaluating it in the vacuum state yields

$$\begin{aligned} &\left(i\,\hbar\,\frac{\partial}{\partial t} - \epsilon_m\left(\frac{q}{2}+k\right) - \epsilon_n\left(\frac{q}{2}-k\right) \right) G_{m,n,s,t}(q;k,t;k',t') \\ &= \delta(t-t')\ \delta_{n,s}\ \delta_{m,t}\ \delta_{\underline{k},\underline{k}'} \\ &\quad + \langle \mid \hat{T}\ \Big[\ \gamma_{m,\frac{q}{2}+k,\sigma}(t)\ \gamma_{n,\frac{q}{2}-k,\overline{\sigma}}(t)\ ,\ \hat{H}_{int}(t)\ \Big]\ \gamma^{\dagger}_{s,\frac{q}{2}-k',\overline{\sigma}}(t')\ \gamma^{\dagger}_{t,\frac{q}{2}+k',\sigma}(t') \mid \rangle \end{aligned} \tag{20}$$

The term involving the commutator is non-zero only if $t-t' > 0$, and is evaluated by putting it into normal ordered form. The result is

$$\sum_{\alpha} A^{\alpha}_{m}\left(\frac{q}{2}+k\right) A^{\alpha}_{n}\left(\frac{q}{2}-k\right) \frac{U}{N} \sum_{s',t',\underline{k}''} A^{\alpha}_{m'}\left(\frac{q}{2}+k''\right) A^{\alpha}_{n'}\left(\frac{q}{2}-k''\right) G_{m',n',s,t}(q;k'',t,k',t') \tag{21}$$

Therefore, we can Fourier transform the equation of motion to obtain

$$\left(\hbar\,\omega - \epsilon_m\left(\frac{q}{2}+k\right) - \epsilon_n\left(\frac{q}{2}-k\right) \right) G_{m,n,s,t}(q,k,k',\omega)$$

$$
\begin{aligned}
&= \delta_{m,t}\ \delta_{n,s}\ \delta_{\underline{k},\underline{k}'} \\
&\quad + \sum_{\alpha}\ A_m^{\alpha}\left(\frac{q}{2}+k\right)\ A_n^{\alpha}\left(\frac{q}{2}-k\right)\ \frac{U}{N}\sum_{\underline{k}'',m',n'}\ A_{m'}^{\alpha}\left(\frac{q}{2}+k''\right)\ A_{n'}^{\alpha}\left(\frac{q}{2}-k''\right)\ G_{m',n',s,t}(q,k'',k',\omega)
\end{aligned}
$$

The Green's function can be rewritten as

$$
\begin{aligned}
& G_{m,n,s,t}(q,k,k',\omega) \\
&= \frac{\delta_{m,t}\ \delta_{n,s}\ \delta_{\underline{k},\underline{k}'}}{\hbar\ \omega\ -\epsilon_m\left(\frac{q}{2}+k\right)-\epsilon_n\left(\frac{q}{2}-k\right)} \\
&\quad + \sum_{\alpha}\ \frac{A_m^{\alpha}\left(\frac{q}{2}+k\right)\ A_n^{\alpha}\left(\frac{q}{2}-k\right)}{\hbar\ \omega\ -\epsilon_m\left(\frac{q}{2}+k\right)-\epsilon_n\left(\frac{q}{2}-k\right)}\ \frac{U}{N}\sum_{\underline{k}'',m',n'}\ A_{m'}^{\alpha}\left(\frac{q}{2}+k''\right)\ A_{n'}^{\alpha}\left(\frac{q}{2}-k''\right)\ G_{m',n',s,t}(q,k'',k',\omega)
\end{aligned}
$$

Defining $C_{s,t}^{\alpha}(k'\omega)$ as

$$
C_{s,t}^{\alpha}(k',\omega) \quad = \quad \sum_{\underline{k}'',m',n'}\ A_{m'}^{\alpha}\left(\frac{q}{2}+k''\right)\ A_{n'}^{\alpha}\left(\frac{q}{2}-k''\right)\ G_{m',n',s,t}(q,k'',k',\omega) \tag{22}
$$

With this notation, the Green's function is given by

$$
\begin{aligned}
& G_{m,n,s,t}(q,k,k',\omega) \\
&= \frac{\delta_{m,t}\ \delta_{n,s}\ \delta_{\underline{k},\underline{k}'}}{\hbar\ \omega\ -\epsilon_m\left(\frac{q}{2}+k\right)-\epsilon_n\left(\frac{q}{2}-k\right)} \\
&\quad + \frac{U}{N}\ \sum_{\alpha}\ \frac{A_m^{\alpha}\left(\frac{q}{2}+k\right)\ A_n^{\alpha}\left(\frac{q}{2}-k\right)}{\hbar\ \omega\ -\epsilon_m\left(\frac{q}{2}+k\right)-\epsilon_n\left(\frac{q}{2}-k\right)}\ C_{s,t}^{\alpha}(q,k',\omega)
\end{aligned}
$$

Then on multiplying the Green's function by $A_m^{\beta}\left(\frac{q}{2}+k\right)\ A_n^{\beta}\left(\frac{q}{2}-k\right)$ and summing over m,n and k, we obtain

$$
\begin{aligned}
& C_{s,t}^{\beta}(q,k',\omega) \\
&= \frac{A_t^{\beta}\left(\frac{q}{2}+k'\right)\ A_s^{\beta}\left(\frac{q}{2}-k'\right)}{\hbar\ \omega\ -\epsilon_t\left(\frac{q}{2}+k'\right)-\epsilon_s\left(\frac{q}{2}-k'\right)} \\
&\quad + \frac{U}{N}\ \sum_{\alpha}\ \sum_{m,n,\underline{k}}\ \frac{A_m^{\alpha}\left(\frac{q}{2}+k\right)A_m^{\beta}\left(\frac{q}{2}+k\right)\ A_n^{\alpha}\left(\frac{q}{2}-k\right)A_n^{\beta}\left(\frac{q}{2}-k\right)}{\hbar\ \omega\ -\epsilon_m\left(\frac{q}{2}+k\right)-\epsilon_n\left(\frac{q}{2}-k\right)}\ C_{s,t}^{\alpha}(q,k',\omega)
\end{aligned} \tag{23}
$$

On defining the correlation function $\Lambda^{\alpha\beta}(\underline{q},\omega)$ by

$$
\Lambda^{\alpha,\beta}(\underline{q},\omega) \quad = \quad \frac{1}{N}\ \sum_{\underline{k},m,n}\ \frac{A_m^{\alpha}\left(\frac{q}{2}+k\right)A_m^{\beta}\left(\frac{q}{2}+k\right)\ A_n^{\alpha}\left(\frac{q}{2}-k\right)A_n^{\beta}\left(\frac{q}{2}-k\right)}{\hbar\ \omega\ -\epsilon_m\left(\frac{q}{2}+k\right)-\epsilon_n\left(\frac{q}{2}-k\right)} \tag{24}
$$

the coupled algebraic equations for C become

$$\begin{aligned} C^{\beta}_{s,t}(q,k',\omega) &= \frac{A^{\beta}_{t}\left(\frac{q}{2}+k'\right)\ A^{\beta}_{s}\left(\frac{q}{2}-k'\right)}{\hbar\ \omega\ -\epsilon_t\left(\frac{q}{2}+k'\right)-\epsilon_s\left(\frac{q}{2}-k'\right)} \\ &\quad + U\ \sum_{\alpha}\Lambda^{\beta,\alpha}(\underline{q},\omega)\ C^{\alpha}_{s,t}(q,k',\omega) \end{aligned} \tag{25}$$

This is a matrix equation

$$\begin{aligned} \sum_{\beta}\ \left(\ \delta^{\alpha,\beta}-U\ \Lambda^{\alpha,\beta}(q,\omega)\ \right)\ C^{\beta}_{s,t}(q,k',\omega) &= \frac{A^{\alpha}_{t}\left(\frac{q}{2}+k'\right)\ A^{\alpha}_{s}\left(\frac{q}{2}-k'\right)}{\hbar\ \omega\ -\epsilon_t\left(\frac{q}{2}+k'\right)-\epsilon_s\left(\frac{q}{2}-k'\right)} \\ &= B^{\alpha}_{s,t}(q,k',\omega) \end{aligned} \tag{26}$$

where we have defined

$$B^{\alpha}_{s,t}(q,k',\omega) = \frac{A^{\alpha}_{t}\left(\frac{q}{2}+k'\right)\ A^{\alpha}_{s}\left(\frac{q}{2}-k'\right)}{\hbar\ \omega\ -\epsilon_t\left(\frac{q}{2}+k'\right)-\epsilon_s\left(\frac{q}{2}-k'\right)} \tag{27}$$

This can be solved using matrix inversion

$$\begin{pmatrix} C^{a}_{s,t} \\ C^{b}_{s,t} \\ C^{c}_{s,t} \end{pmatrix} = \frac{1}{Det(q,\omega)} \begin{pmatrix} \Gamma^{aa}(q,\omega) & \Gamma^{ab}(q,\omega) & \Gamma^{ac}(q,\omega) \\ \Gamma^{ba}(q,\omega) & \Gamma^{bb}(q,\omega) & \Gamma^{bc}(q,\omega) \\ \Gamma^{ca}(q,\omega) & \Gamma^{cb}(q,\omega) & \Gamma^{cc}(q,\omega) \end{pmatrix} \begin{pmatrix} B^{a}_{s,t} \\ B^{b}_{s,t} \\ B^{c}_{s,t} \end{pmatrix}$$

where the determinant of the matrix is given by

$$\begin{aligned} Det(q,\omega) &= (1-U\Lambda^{aa}(q,\omega))(1-U\Lambda^{bb}(q,\omega))(1-U\Lambda^{cc}(q,\omega)) \\ &\quad -(1-U\Lambda^{aa}(q,\omega))\ \left(\ U\ \Lambda^{bc}(q,\omega)\ \right)^2 \\ &\quad -(1-U\Lambda^{bb}(q,\omega))\ \left(\ U\ \Lambda^{ac}(q,\omega)\ \right)^2 \\ &\quad -(1-U\Lambda^{cc}(q,\omega))\ \left(\ U\ \Lambda^{ab}(q,\omega)\ \right)^2 \\ &\quad -2\ U^3\ \Lambda^{ab}(q,\omega)\ \Lambda^{bc}(q,\omega)\ \Lambda^{ca}(q,\omega) \end{aligned} \tag{28}$$

and the transposed matrix of cofactors is

$$\begin{aligned} \Gamma^{a,a}(q,\omega) &= (1-U\Lambda^{bb}(q,\omega))(1-U\Lambda^{cc}(q,\omega)) - \left(\ U\ \Lambda^{bc}(q,\omega)\ \right)^2 \\ \Gamma^{b,b}(q,\omega) &= (1-U\Lambda^{aa}(q,\omega))(1-U\Lambda^{cc}(q,\omega)) - \left(\ U\ \Lambda^{ac}(q,\omega)\ \right)^2 \\ \Gamma^{c,c}(q,\omega) &= (1-U\Lambda^{aa}(q,\omega))(1-U\Lambda^{bb}(q,\omega)) - \left(\ U\ \Lambda^{ab}(q,\omega)\ \right)^2 \\ \Gamma^{a,b}(q,\omega) &= (1-U\Lambda^{cc}(q,\omega))\ U\ \Lambda^{ba}(q,\omega) + U^2\ \Lambda^{bc}(q,\omega)\ \Lambda^{ca}(q,\omega) \\ \Gamma^{a,c}(q,\omega) &= (1-U\Lambda^{bb}(q,\omega))\ U\ \Lambda^{ac}(q,\omega) + U^2\ \Lambda^{ab}(q,\omega)\ \Lambda^{bc}(q,\omega) \\ \Gamma^{b,c}(q,\omega) &= (1-U\Lambda^{aa}(q,\omega))\ U\ \Lambda^{bc}(q,\omega) + U^2\ \Lambda^{ab}(q,\omega)\ \Lambda^{ca}(q,\omega) \end{aligned} \tag{29}$$

In general, for an asymmetric matrix with elements $M^{\alpha,\beta}$ then

$$\Gamma^{\alpha,\beta} = \frac{\partial Det}{\partial M^{\beta,\alpha}} \tag{30}$$

in which the order of the indices need to be strictly retained. The gradient of $\det M$ with respect to the matrix M is the transpose of the matrix of cofactors. To summarize, we have determined that

$$C^{\alpha}_{s,t}(q,k',\omega) \;=\; \frac{1}{Det(q,\omega)} \sum_{\beta} \Gamma^{\alpha,\beta}(q,\omega)\; B^{\beta}_{s,t}(q,k',\omega) \tag{31}$$

The Green's function can then be expressed as

$$\begin{aligned} G_{m,n,s,t}(q,k,k',\omega) \;=\; & \frac{\delta_{m,t}\;\delta_{n,s}\;\delta_{k,k'}}{\hbar\omega \;-\epsilon_s\left(\frac{q}{2}-k\right)-\epsilon_t\left(\frac{q}{2}+k\right)} \\ & + \sum_{\alpha} B^{\alpha}_{m,n}(q,k,\omega)\;\frac{U}{N}\;C^{\alpha}_{st}(q,k',\omega) \end{aligned} \tag{32}$$

Inserting the expression for $C^{\alpha}_{s,t}$, one finds

$$\begin{aligned} G_{m,n,s,t}(q,k,k',\omega) \;=\; & \frac{\delta_{m,t}\;\delta_{n,s}\;\delta_{k,k'}}{\hbar\omega \;-\epsilon_s\left(\frac{q}{2}-k\right)-\epsilon_t\left(\frac{q}{2}+k\right)} \\ & + \frac{U}{N}\sum_{\alpha,\beta} B^{\alpha}_{m,n}(q,k,\omega)\;\frac{\Gamma^{\alpha,\beta}(q,\omega)}{Det(q,\omega)}\;B^{\beta}_{s,t}(q,k',\omega) \end{aligned} \tag{33}$$

This may be written as

$$\begin{aligned} G_{m,n,s,t}(q,k,k',\omega) \;=\; & \delta_{m,t}\;\delta_{n,s}\;\delta_{k,k'}\;G^{0}_{m,n}(q,k,\omega) \\ & + G^{0}_{m,n}(q,k,\omega)\;T_{m,n,s,t}(q,k,k',\omega)\;G^{0}_{s,t}(q,k',\omega) \end{aligned} \tag{34}$$

where the non-interacting Green's function is given by

$$G^{0}_{m,n}(q,k,\omega) \;=\; \frac{1}{\hbar\omega \;-\epsilon_n\left(\frac{q}{2}-k\right)-\epsilon_m\left(\frac{q}{2}+k\right)} \tag{35}$$

and where the T-matrix is expressed as

$$T_{m,n,s,t}(q,k,k',\omega) \;=\; \frac{U}{N}\sum_{\alpha,\beta} A^{\alpha}_{m}\left(\frac{q}{2}+k\right)\;A^{\alpha}_{n}\left(\frac{q}{2}-k\right)\frac{\Gamma^{\alpha,\beta}(q,\omega)}{Det(q,\omega)}A^{\beta}_{t}\left(\frac{q}{2}+k'\right)\;A^{\beta}_{s}\left(\frac{q}{2}-k'\right)$$

5 The Density of States

The two-electron density of states, with center of mass momentum q is given by the imaginary part of the Trace of the Green's Function.

$$\rho(q,\omega) \;=\; -\frac{1}{\pi}\;\frac{1}{N}\sum_{k,m,n} \Im m\; G_{m,n,n,m}(q,k,k,\omega)$$

$$
\begin{aligned}
&= \frac{1}{N}\sum_{m,n,k}\delta\Big(\ \hbar\omega-\epsilon_m\left(\frac{q}{2}+k\right)-\epsilon_n\left(\frac{q}{2}-k\right)\ \Big)\\
&\quad -\frac{1}{N\ \pi}\,\Im m\ \sum_{\alpha,\beta}\ \frac{1}{Det(q,\omega)}\ \frac{U}{N}\ \sum_{k,m,n}\ B^{\alpha}_{m,n}(q,k,\omega)\ \Gamma^{\alpha,\beta}(q,\omega)\ B^{\beta}_{m,n}(q,k,\omega)\\
&= \frac{1}{N}\sum_{m,n,k}\delta\Big(\ \hbar\omega-\epsilon_m\left(\frac{q}{2}+k\right)-\epsilon_n\left(\frac{q}{2}-k\right)\ \Big)\\
&\quad +\frac{1}{N\ \pi}\,\Im m\ \sum_{\alpha,\beta}\ \frac{U}{Det(q,\omega)}\ \frac{\partial\Lambda^{\alpha,\beta}(\omega)}{\hbar\partial\omega}\ \Gamma^{\alpha,\beta}(q,\omega)\\
&= \frac{1}{N}\sum_{m,n,k}\delta\Big(\ \hbar\omega-\epsilon_m\left(\frac{q}{2}+k\right)-\epsilon_n\left(\frac{q}{2}-k\right)\ \Big)\\
&\quad -\frac{1}{N\ \pi}\,\Im m\ \sum_{\alpha,\beta}\ \frac{1}{Det(q,\omega)}\ \frac{\partial(\delta^{\alpha,\beta}-U\Lambda^{\alpha,\beta}(q,\omega))}{\hbar\partial\omega}\frac{\partial Det(q,\omega)}{\partial(\delta^{\alpha,\beta}-U\Lambda^{\alpha,\beta}(q,\omega))}\\
&= \frac{1}{N}\sum_{m,n,k}\delta\Big(\ \hbar\omega-\epsilon_m\left(\frac{q}{2}+k\right)-\epsilon_n\left(\frac{q}{2}-k\right)\ \Big)-\frac{1}{N\ \pi}\,\Im m\ \frac{\partial\ln Det(q,\omega)}{\hbar\partial\omega}\\
&= \rho^0(q,\omega)\ -\frac{\Im m}{N\ \pi}\ \frac{\partial\ln Det(q,\omega)}{\partial\hbar\omega}\\
&= \rho^0(q,\omega)\ -\ \frac{1}{N\ \pi}\ \frac{\partial\ \delta(q,\omega)}{\partial\hbar\omega} \qquad (36)
\end{aligned}
$$

The first term is the non-interacting two-electron density of states and the second term is the change in the density of states due to the interaction which is written as the derivative of the phase of the T-Matrix, $\delta(q,\omega)$, defined by

$$
\delta(q,\omega) \quad = \quad \Im m\ \ln Det(q,\omega) \qquad (37)
$$

In accordance with Levinson's theorem, the T-matrix contribution maintains unitarity.

Alternatively, one may express the density of states as

$$
\begin{aligned}
\rho(q,\omega) &= \rho^0(q,\omega)-\frac{\Im m}{\pi}\ \frac{U}{N}\ \sum_{\alpha,\beta,k}\ \frac{\Gamma^{\alpha,\beta}(q,\omega)}{Det(q,\omega)}\frac{A^{\alpha}_m\left(\frac{q}{2}+k\right)A^{\beta}_m\left(\frac{q}{2}+k\right)\ A^{\alpha}_n\left(\frac{q}{2}-k\right)A^{\beta}_n\left(\frac{q}{2}-k\right)}{(\hbar\omega-\epsilon_m\left(\frac{q}{2}+k\right)-\epsilon_n\left(\frac{q}{2}-k\right))^2}\\
&= \rho^0(q,\omega)+\frac{\Im m}{\pi}\ \frac{U}{N}\ \sum_{\alpha,\beta}\ \frac{\Gamma^{\alpha,\beta}(q,\omega)}{Det(q,\omega)}\ \frac{\partial\Lambda^{\alpha,\beta}(q,\omega)}{\partial\hbar\omega}\\
&= \rho^0(q,\omega)-\frac{\Im m}{N\ \pi}\ \sum_{\alpha,\beta}\ \frac{\Gamma^{\alpha,\beta}(q,\omega)}{Det(q,\omega)}\ \frac{\partial}{\partial\hbar\omega}\Big[\ \delta^{\alpha,\beta}-U\Lambda^{\alpha,\beta}(q,\omega)\ \Big]\\
&= \rho_0(q,\omega)\ +\ \Delta\rho(q,\omega) \qquad (38)
\end{aligned}
$$

As a check of the results, one may examine the atomic limit for which the off-diagonal site correlation functions vanish, and the diagonal correlation functions reduced to

$$\Lambda^{\alpha,\alpha}(q,\omega) \;=\; \frac{1}{\hbar\omega} \tag{39}$$

Hence,

$$Det(q,\omega) \;=\; \left(\; 1 \; - \; \frac{U}{\hbar\omega} \; \right)^3 \tag{40}$$

In this limit, the non-interacting two-electron density of states is given by

$$\begin{aligned} \rho_0(q,\omega) \;&=\; -\frac{1}{N\pi} \; \Im m \; \left[\frac{9N}{\hbar\omega} \right] \\ &=\; 9 \; \delta(\hbar\omega) \end{aligned} \tag{41}$$

The total density of states is evaluated as

$$\begin{aligned} \rho(q,\omega) \;&=\; \rho_0(q,\omega) \; - \; \frac{\Im m}{N\pi} \left[\; \frac{\partial}{\partial\hbar\omega} \; \ln \; Det(q,\omega) \; \right] \\ &=\; 9 \; \delta(\omega) \; - \frac{3}{N \; \pi} \; \Im m \left[\frac{1}{\hbar\omega - U} \; - \frac{1}{\hbar\omega} \; \right] \\ &=\; \frac{9N-3}{N} \; \delta(\hbar\omega) \; + \; \frac{3}{N} \; \delta(\hbar\omega - U) \end{aligned} \tag{42}$$

Physically, this has an interpretation that if the pair of electrons are distributed onto the $3N$ sites of the lattice, there are 3 N possibilities that the sites are doubly occupied and have excitation energy U while the remaining $(9N^2 - 3N)$ configurations have their sites singly occupied and do not experience the Coulomb interaction. Since we have normalized the two-particle density of states with center of mass momentum q by the number of unit cells N and since there are N values of q, the weights of the two spectral features appear as $\frac{9N-3}{N}$ and $\frac{3}{N}$, respectively.

For future reference, we note that, in the atomic limit, the phase shift is given by

$$\delta(q,\omega) \;=\; 3 \; \pi \; [\; \Theta(\hbar\omega) \; - \; \Theta(\hbar\omega - U) \;] \tag{43}$$

which is independent of q.

Using Eqn. (**??**), in Fig.(**??**) we plot the non-interacting two-electron density of states $\rho_0(q,\omega)$ of the Lieb lattice, with the center of mass momentum $\underline{q}$ at special points of the Brillouin zone: Γ, X and M. Likewise, in Fig.(4) we plot the change in the density of states $\Delta\rho(q,\omega)$ due to the interaction at various points in the Brillouin zone.

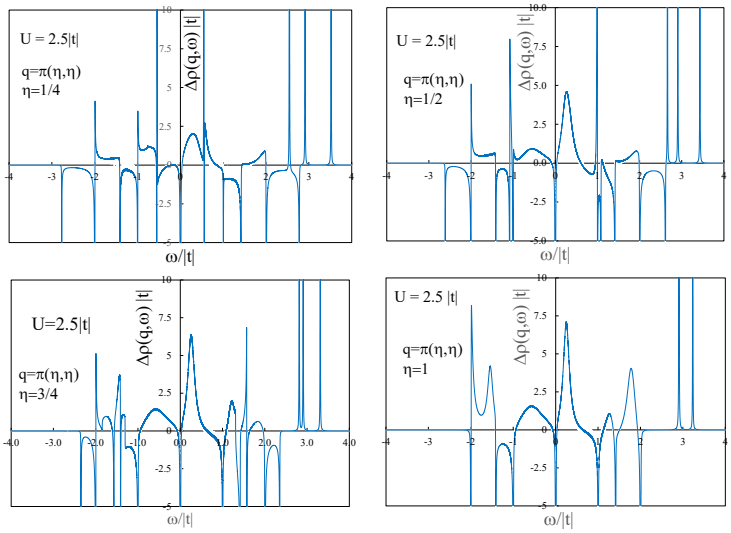

Figure 4: The frequency dependence of the T-Matrix contribution to the density of states $\Delta\rho(q,\omega)$ for $U = 2.5|t|$ with center of mass momenta $q = \pi(\eta,\eta)$ with $\eta = 0.25,\ 0.5,\ 0.75$ and 1.

5.1 Spectral Sum Rules

The two-electron density of states, with center of mass momentum q has moments defined as

$$\begin{aligned} M_n(q) &= \int_{-\infty}^{\infty} d\omega\ \hbar^{n+1}\ \omega^n\ \rho(q,\omega) \\ &= \int_{-\infty}^{\infty} d\omega\ \hbar^{n+1}\ \omega^n\ \Big[\ \rho_0(q,\omega)\ +\ \Delta\rho(q,\omega)\ \Big] \end{aligned} \tag{44}$$

For the non-interacting density of states, one finds the moments are given by

$$\begin{aligned} M_0^0(q) &= 9 \\ M_1^0(q) &= 0 \\ M_2^0(q) &= 12\ |t|^2 \\ M_3^0(q) &= 0 \\ M_4^0(q) &= 3\ |t|^4\ (\ 13\ +\ \cos q_x\ +\ \cos q_y\ ) \\ M_5^0(q) &= 0 \end{aligned} \tag{45}$$

for all q values. The odd moments vanish since the chiral operator anti-commutes with the non-interacting Bloch Hamiltonian. For the case where U is finite, then due to unitarity and conservation of center of mass momentum $M_0^0(q)$ is independent of q. The moments can be expressed as

$$M_n(q) \ = \ M_n^0(q)\ +\ \Delta M_n(q) \tag{46}$$

where $M_n(q)$ is the moment associated with the T-Matrix contribution to the two-electron spectral density. This can be written as

$$\begin{aligned}
\Delta M_n(q) &= -\frac{\Im m}{N\ \pi}\ \left[\ \hbar^n \omega^n\ \ln Det(q,\omega)\ \Big|_{-\infty}^{\infty} -\ n\ \int_{-\infty}^{\infty} d\omega\ \hbar^n\ \omega^{n-1}\ \ln Det(q,\omega)\ \right] \\
&= n\ \frac{\Im m}{N\ \pi}\ \left[\ \int_{-\infty}^{\infty} d\omega\ \hbar^n\ \omega^{n-1}\ \ln Det(q,\omega)\ \right] \\
&= \frac{n}{N\ \pi}\ \int_{-\infty}^{\infty} d\omega\ \hbar^n\ \omega^{n-1}\ \delta(q,\omega) \qquad (47)
\end{aligned}$$

The boundary term in the first line vanished identically since

$$\lim_{|\omega|\to\infty}\ \Im m\ Det(q,\omega) \ \ \to\ \ 0 \qquad (48)$$

and

$$\lim_{|\omega|\to\infty}\ \Re e\ Det(q,\omega) \ \ \to\ \ 1 \qquad (49)$$

which causes the phase shift to vanish.

The moments $\Delta M_n(q)$ characterize the change in the two-electron spectral density due to the Coulomb interaction U and are a measure of the asymmetry of the two-electron spectra. Since the Trace of the interaction, in the subspace of two-electron states with center of mass momentum q, is given by

$$\sum_{k,m,n}\ \langle\ \frac{q}{2}+k,m;\frac{q}{2}-k,n\ \mid\ \hat{H}_{int}\ \mid\ \frac{q}{2}+k,m;\frac{q}{2}-k,n\ \rangle\ \ =\ \ \frac{U}{N}\sum_{k,m,n,\alpha}\ |A_m^\alpha\left(\frac{q}{2}+k\right)|^2\ |A_n^\alpha\left(\frac{q}{2}-k\right)|^2 \qquad (50)$$

one may use the cyclic invariance of the trace and the orthogonality relations

$$\sum_n\ A_n^\alpha\left(\frac{q}{2}\pm k\right)\ A_n^\beta\left(\frac{q}{2}\pm k\right)\ \ =\ \ \delta^{\alpha,\beta} \qquad (51)$$

to show that

$$\begin{aligned}
\Delta M_1(q) &= 3\ \frac{U}{N} \\
\Delta M_2(q) &= 3\ \frac{U^2}{N} \\
\Delta M_3(q) &= 3\ \frac{U^3}{N}\ +\ 12\ |t|^2\ \frac{U}{N} \\
\Delta M_4(q) &= 3\ \frac{U^4}{N}\ +\ 12\ |t|^2\ \frac{U^2}{N} \\
\Delta M_5(q) &= 3\ \frac{U^5}{N}\ +\ 20\ |t|^2\ \frac{U^3}{N}\ +\ \frac{5}{2}\ |t|^4\ \frac{U}{N}\ [\ 28\ +\ 3\ (\ \cos q_x\ +\ \cos q_y\ )\ ] \\
\Delta M_6(q) &= 3\ \frac{U^6}{N}\ +\ 24\ |t|^2\ \frac{U^4}{N}\ +\ 3\ |t|^4\ \frac{U^2}{N}\ [\ 66\ +\ 19\ (\cos q_x\ +\ \cos q_y\ )\ ]
\end{aligned} \qquad (52)$$

The first term in these expressions matches the values found in the atomic limit.

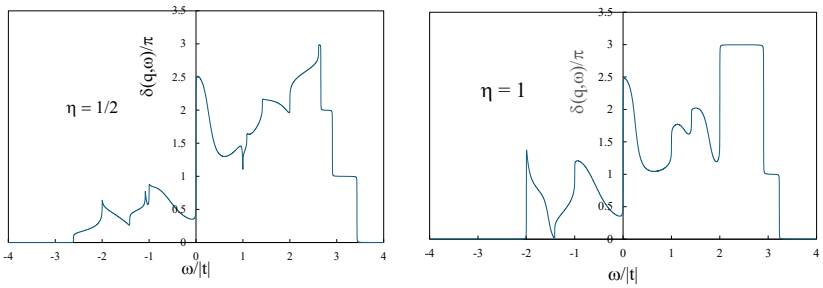

Figure 5: The frequency-dependent phase shift $\delta(q,\omega)/\pi$ evaluated for $q = \pi/2(1,1)$ and $q = \pi(1,1)$ with $U = 2.5|t|$. It is seen that the difference in the value of the phase shift between the edges of the continuum has a magnitude of 3π, which indicates the presence of three bound states at excitation energies $\hbar\,\omega\ \sim U$.

The moments calculated from the frequency dependent phase-shift for $q = \pi(0.5, 0.5)$ and $U = 2.5\ |t|$ [shown in Fig. (5)] yield

$$\begin{aligned}
\Delta M_0(q) &= 0 \\
\Delta M_1(q) &= \frac{7.498}{N} \\
\Delta M_2(q) &= \frac{18.743}{N} \\
\Delta M_3(q) &= \frac{76.879}{N} \\
\Delta M_4(q) &= \frac{217.183}{N} \\
\Delta M_5(q) &= \frac{780.931}{N}
\end{aligned} \tag{53}$$

to be compared with the analytic expression 7.5, 18.75, 76.875, 192.1875 and 817.969. The moments calculated numerically (Marcos with N=81) from $\Delta\rho(q,\omega)$ for $U = 2|t|$ at $q = (0,0)$ are

$$\begin{aligned}
\Delta M_0(q) &= 0 \\
\Delta M_1(q) &= \frac{5.994}{N} \\
\Delta M_2(q) &= \frac{10.692}{N} \\
\Delta M_3(q) &= \frac{43.092}{N} \\
\Delta M_4(q) &= \frac{100.683}{N} \\
\Delta M_5(q) &= \frac{396.739}{N}
\end{aligned} \tag{54}$$

compared to the analytic expressions 6, 12, 48, 96 and 426. The numerically calculated higher order moments are larger and will yield poorer agreement with the analytic expressions, since instead of evaluating a sum over delta functions the spectral density is being represented by a sum of Lorentzians, so the integrands for large ω has a frequency variation $\sim\ \omega^n\ \frac{\eta}{(\omega-\epsilon_0)^2+\eta^2}$ which diverges for $n > 2$ like $\frac{\eta}{n}\ \omega^{n-1}$ when $\omega \to \infty$. Consequently, one expects that the long high energy tails provide spurious excess contributions to the sum rule.

5.2 The Central Peak

The two-electron excitation spectral density has a peak at $\omega = 0$. The non-interacting spectrum has three contributions near $\omega = 0$, given by

$$\begin{aligned}\rho_0(q,\omega) &= \delta(\hbar\omega) + \frac{1}{N}\sum_k \Big[\ \delta\left(\hbar\omega - \epsilon_+\left(\frac{q}{2}+k\right) - \epsilon_-\left(\frac{q}{2}-k\right)\right) \\ &\quad + \delta\left(\hbar\omega - \epsilon_-\left(\frac{q}{2}+k\right) - \epsilon_+\left(\frac{q}{2}-k\right)\right)\ \Big] \qquad (55)\end{aligned}$$

Thus, the central peak of the non-interacting spectral density has a q-independent contribution of weight unity due to the flat band and a symmetric peak with a q-dependent width given by $\Delta\omega(q) = |t|\ \sqrt{\sin^2\frac{q_x}{2} + \sin^2\frac{q_y}{2}}$, which reduces to a delta function of strength 2 when $q \to 0$. The central peak can be approximated as

$$\begin{aligned}\rho_0(q,\omega) &\approx \delta(\hbar\omega) + \frac{2}{\hbar\Delta\omega(q)}\,\Theta(\,\Delta\omega(q) - |\omega|\,)\ \Big[\ -\ A\ \ln\left(\frac{|\omega|}{\Delta\omega(q)}\right) \\ &\quad + \frac{2\ B}{\pi}\ \sqrt{1-\left(\frac{\omega}{\Delta\omega(q)}\right)^2}\ \Big] \qquad (56)\end{aligned}$$

and is shown in Fig.(6) for $q = \pi(0.05, 0.05)$.

The correlation functions $\Lambda^{\alpha,\beta}(q,\omega)$ have singularities at $\omega = 0$ with the asymptotic forms

$$\begin{aligned}\Lambda^{a,a}(q,\omega) &= \Delta\Lambda^{a,a}(q,\omega) \\ \Lambda^{a,b}(q,\omega) &= \Delta\Lambda^{a,b}(q,\omega) \\ \Lambda^{a,c}(q,\omega) &= \Delta\Lambda^{a,c}(q,\omega) \\ \Lambda^{b,b}(q,\omega) &= \frac{F^{b,b}(q)}{\hbar\omega} + \Delta\Lambda^{b,b}(q,\omega) \\ \Lambda^{c,c}(q,\omega) &= \frac{F^{c,c}(q)}{\hbar\omega} + \Delta\Lambda^{c,c}(q,\omega) \\ \Lambda^{b,c}(q,\omega) &= \frac{F^{b,c}(q)}{\hbar\omega} + \Delta\Lambda^{b,c}(q,\omega) \qquad (57)\end{aligned}$$

where

$$F^{b,b}(q) = \frac{1}{N}\sum_k \left[\frac{(1+\cos\frac{q_x}{2}\cos k_x)^2 - (\sin\frac{q_x}{2}\sin k_x)^2}{(2+\cos\frac{q_x}{2}\cos k_x + \cos\frac{q_y}{2}\cos k_y)^2 - (\sin\frac{q_x}{2}\sin k_x + \sin\frac{q_y}{2}\sin k_y)^2}\right]$$

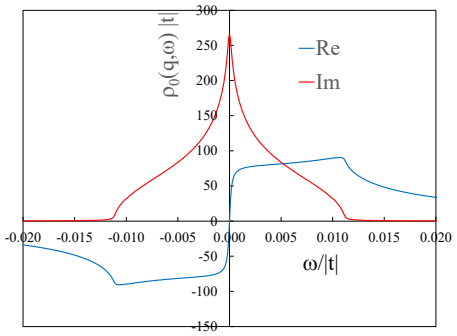

Figure 6: The frequency dependence of the non-interacting central peak for $q = \pi(0.05, 0.05)$ which shows a logarithmic cusp at $\omega = 0$, and a width of $2\Delta\omega(q)$.

$$F^{c,c}(q) = \frac{1}{N}\sum_k \left[\frac{(1+\cos\frac{q_y}{2}\cos k_y)^2 - (\sin\frac{q_y}{2}\sin k_y)^2}{(2+\cos\frac{q_x}{2}\cos k_x + \cos\frac{q_y}{2}\cos k_y)^2 - (\sin\frac{q_x}{2}\sin k_x + \sin\frac{q_y}{2}\sin k_y)^2}\right]$$
$$F^{b,c}(q) = \frac{1}{N}\sum_k \left[\frac{(\cos\frac{q_x}{2}+\cos k_x)\,(\cos\frac{q_y}{2}+\cos k_y)}{(2+\cos\frac{q_x}{2}\cos k_x + \cos\frac{q_y}{2}\cos k_y)^2 - (\sin\frac{q_x}{2}\sin k_x + \sin\frac{q_y}{2}\sin k_y)^2}\right] \tag{58}$$

Hence, for real frequencies, the asymptotic $\omega \to 0$ limit of the determinant is given by

$$Det(q,\omega) = (1 - U\Delta\Lambda^{a,a}(q,\omega))\left(\frac{U}{\hbar\omega}\right)^2 \left(F^{b,b}F^{c,c} - F^{b,c\ 2}\right) \tag{59}$$

The corresponding asymptotic limit of the derivative of the determinant is

$$\frac{\partial Det(q,\omega)}{\partial\omega} = \left[-\frac{2}{\omega}\,(1 - U\Delta\Lambda^{a,a}(q,\omega)) + U\,\frac{\partial\Lambda^{a,a}(q,\omega)}{\partial\omega}\right]\left(\frac{U}{\hbar\omega}\right)^2 \left(F^{b,b}F^{c,c} - F^{b,c\ 2}\right) \tag{60}$$

The non-interacting two-electron flat band state is N-fold degenerate and is composed of linear combinations of the states

$$\left[\cos\left(\frac{q_y+2k_y}{4}\right) b^\dagger_{\frac{q}{2}+k,\sigma} - \cos\left(\frac{q_x+2k_x}{4}\right) c^\dagger_{\frac{q}{2}+k,\sigma}\right]\left[\cos\left(\frac{q_y-2k_y}{4}\right) b^\dagger_{\frac{q}{2}-k,\overline{\sigma}} - \cos\left(\frac{q_x-2k_x}{4}\right) c^\dagger_{\frac{q}{2}-k,\overline{\sigma}}\right] |\ \rangle \tag{61}$$

5.3 Hubbard Band Formation

$$\frac{1}{\sqrt{3\ N}}\sum_k \left(\ a^\dagger_{k,\sigma}a^\dagger_{-k,\overline{\sigma}} - b^\dagger_{k,\sigma}b^\dagger_{-k,\overline{\sigma}} - c^\dagger_{k,\sigma}c^\dagger_{-k,\overline{\sigma}}\ \right) |\ \rangle \tag{62}$$

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6 Work in Progress: The Two-Electron Self-Energy

The T-Matrix expression for the diagonal two-electron Green's function

$$\begin{aligned} G_{m,n,m,n}(q,k,k,\omega) &= G^0_{m,n}(q,k,\omega) \\ &\quad + G^0_{m,n}(q,k,\omega)\ T_{m,n}(q,k,\omega)\ G^0_{m,n}(q,k,\omega) \end{aligned} \tag{63}$$

can also be expressed in terms of the two-electron self-energy

$$\begin{aligned} G_{m,n,m,n}(q,k,k,\omega) &= \frac{1}{G^0_{m,n}(q,k,\omega)^{-1} \ - \ \Sigma_{m,n}(q,k,\omega)} \\ &= \frac{G^0_{m,n}(q,k,\omega)}{1 \ - \ \Sigma_{m,n}(q,k,\omega)\ G^0_{m,n}(q,k,\omega)} \end{aligned} \tag{64}$$

which can be expanded as

$$G_{m,n,m,n}(q,k,k,\omega) = G^0_{m,n}(q,k,\omega) \ + \ G^0_{m,n}(q,k,\omega)\ \Sigma_{m,n}(q,k,\omega)\ G^0_{m,n}(q,k,\omega) \ + \ \ldots \tag{65}$$

Hence, for large N, the self-energy can be approximated by

$$\begin{aligned} \Sigma_{m,n}(q,k,\omega) &= T_{m,n}(q,k,\omega) \\ &= \frac{U}{N} \sum_{\alpha,\beta} A^\alpha_m\left(\frac{q}{2}+k\right)\ A^\beta_m\left(\frac{q}{2}+k\right)\ \frac{\Gamma^{\alpha,\beta}(q,\omega)}{Det(q,\omega)}\ A^\alpha_n\left(\frac{q}{2}-k\right)\ A^\beta_n\left(\frac{q}{2}-k\right) \end{aligned}$$

since the corrections are of higher-order in $\frac{1}{N}$. Since the poles of the two-electron Green's function lead to the identification of the two-electron quasi-particle excitation energies and their lifetimes, the self-energy encapsulates the contribution

due to the interactions.

The determinant of the matrix is given by

$$\begin{aligned} Det(q,\omega) &= (1-U\Lambda^{aa}(q,\omega))(1-U\Lambda^{bb}(q,\omega))(1-U\Lambda^{cc}(q,\omega)) \\ &\quad - (1-U\Lambda^{aa}(q,\omega))\ \left(\ U\ \Lambda^{bc}(q,\omega)\ \right)^2 \\ &\quad - (1-U\Lambda^{bb}(q,\omega))\ \left(\ U\ \Lambda^{ac}(q,\omega)\ \right)^2 \\ &\quad - (1-U\Lambda^{cc}(q,\omega))\ \left(\ U\ \Lambda^{ab}(q,\omega)\ \right)^2 \\ &\quad - 2\ U^3\ \Lambda^{ab}(q,\omega)\ \Lambda^{bc}(q,\omega)\ \Lambda^{ca}(q,\omega) \end{aligned} \tag{66}$$

and the real and imaginary parts of the $\Gamma^{\alpha,\beta}$ are found as:

$$\begin{aligned} \Re e\ \Gamma^{a,a}(q,\omega) &= (1-U\Re e\ \Lambda^{bb}(q,\omega))(1-U\Re e\ \Lambda^{cc}(q,\omega)) - \left(\ U\ \Re e\ \Lambda^{bc}(q,\omega)\ \right)^2 \\ &\quad - U^2\ \left[\ \Im m\ \Lambda^{bb}(q,\omega)\ \Im m\ \Lambda^{cc}(q,\omega)\ -\ \Im m\ \Lambda^{bc}(q,\omega)^2\ \right] \\ \Im m\ \Gamma^{a,a}(q,\omega) &= -\ U\ \Im m\ \Lambda^{bb}(q,\omega)\ (1-U\Re e\ \Lambda^{cc}(q,\omega)) - U\ \Im m\ \Lambda^{cc}(q,\omega)\ (1-U\Re e\ \Lambda^{bb}(q,\omega)) \\ &\quad - 2\ U^2\ \Im m\ \Lambda^{bc}(q,\omega)\ \Re e\ \Lambda^{bc}(q,\omega) \\ \Re e\ \Gamma^{b,b}(q,\omega) &= (1-U\Re e\Lambda^{aa}(q,\omega))(1-U\Re e\Lambda^{cc}(q,\omega)) - (\ U\ \Re e\ \Lambda^{ac}(q,\omega)\ )^2 \\ &\quad - U^2\ \left[\ \Im m\ \Lambda^{aa}(q,\omega)\ \Im m\ \Lambda^{cc}(q,\omega)\ -\ \Im m\ \Lambda^{ac}(q,\omega)^2\ \right] \\ \Im m\ \Gamma^{b,b}(q,\omega) &= -\ U\ \Im m\ \Lambda^{aa}(q,\omega)\ (1-U\Re e\ \Lambda^{cc}(q,\omega)) - U\ \Im m\ \Lambda^{cc}(q,\omega)\ (1-U\Re e\ \Lambda^{aa}(q,\omega)) \\ &\quad - 2\ U^2\ \Im m\ \Lambda^{ac}(q,\omega)\ \Re e\ \Lambda^{ac}(q,\omega) \\ \Re e\ \Gamma^{c,c}(q,\omega) &= (1-U\Re e\Lambda^{aa}(q,\omega))(1-U\Re e\Lambda^{bb}(q,\omega)) - \left(\ U\ \Re e\ \Lambda^{ab}(q,\omega)\ \right)^2 \\ &\quad - U^2\ \left[\ \Im m\ \Lambda^{aa}(q,\omega)\ \Im m\ \Lambda^{bb}(q,\omega)\ -\ \Im m\ \Lambda^{ab}(q,\omega)^2\ \right] \\ \Im m\ \Gamma^{cc}(q,\omega) &= -\ U\ \Im m\ \Lambda^{aa}(q,\omega)\ (1-U\Re e\ \Lambda^{bb}(q,\omega)) - U\ \Im m\ \Lambda^{bb}(q,\omega)\ (1-U\Re e\ \Lambda^{aa}(q,\omega)) \\ &\quad - 2\ U^2\ \Im m\ \Lambda^{ab}(q,\omega)\ \Re e\ \Lambda^{ab}(q,\omega) \\ \Re e\ \Gamma^{a,b}(q,\omega) &= (1-U\Re e\ \Lambda^{cc}(q,\omega))\ U\ \Re e\ \Lambda^{ba}(q,\omega) + U^2\ \Re e\ \Lambda^{bc}(q,\omega)\ \Re e\ \Lambda^{ca}(q,\omega) \\ &\quad + U^2\ \left[\ \Im m\ \Lambda^{cc}(q,\omega)\ \Im m\ \Lambda^{ba}(q,\omega)\ -\ \Im m\ \Lambda^{bc}(q,\omega)\ \Im m\ \Lambda^{ca}(q,\omega)\right] \\ \Im m\ \Gamma^{a,b}(q,\omega) &= (1-U\Re e\ \Lambda^{cc}(q,\omega))\ U\ \Im m\ \Lambda^{ba}(q,\omega)\ -\ U^2\Im m\ \Lambda^{cc}(q,\omega))\ \Re e\ \Lambda^{ba}(q,\omega) \\ &\quad + U^2\ \left[\ \Im m\ \Lambda^{bc}(q,\omega)\ \Re e\ \Lambda^{ca}(q,\omega)\ +\ \Re e\ \Lambda^{bc}(q,\omega)\ \Im m\ \Lambda^{ca}(q,\omega)\ \right] \\ \Re e\ \Gamma^{a,c}(q,\omega) &= (1-U\Re e\ \Lambda^{bb}(q,\omega))\ U\ \Re e\ \Lambda^{ac}(q,\omega) + U^2\ \Re e\ \Lambda^{bc}(q,\omega)\ \Re e\ \Lambda^{ab}(q,\omega) \\ &\quad + U^2\ \left[\ \Im m\ \Lambda^{bb}(q,\omega)\ \Im m\ \Lambda^{ac}(q,\omega)\ -\ \Im m\ \Lambda^{bc}(q,\omega)\ \Im m\ \Lambda^{ab}(q,\omega)\right] \\ \Im m\ \Gamma^{a,c}(q,\omega) &= (1-U\Re e\ \Lambda^{bb}(q,\omega))\ U\ \Im m\ \Lambda^{ac}(q,\omega)\ -\ U^2\Im m\ \Lambda^{bb}(q,\omega))\ \Re e\ \Lambda^{ac}(q,\omega) \\ &\quad + U^2\ \left[\ \Im m\ \Lambda^{bc}(q,\omega)\ \Re e\ \Lambda^{ab}(q,\omega)\ +\ \Re e\ \Lambda^{bc}(q,\omega)\ \Im m\ \Lambda^{ab}(q,\omega)\ \right] \end{aligned}$$

$$
\begin{aligned}
\Re e\ \Gamma^{b,c}(q,\omega) &= (1 - U\Re e\ \Lambda^{aa}(q,\omega))\ U\ \Re e\ \Lambda^{bc}(q,\omega) + U^2\ \Re e\ \Lambda^{ab}(q,\omega)\ \Re e\ \Lambda^{ca}(q,\omega) \\
&\quad + U^2\ \Im m\ \Lambda^{aa}(q,\omega)\ \Im m\ \Lambda^{bc}(q,\omega)\ -\ U^2\ \Im m\ \Lambda^{ab}(q,\omega)\ \Im m\ \Lambda^{ca}(q,\omega) \\
\Im m\ \Gamma^{b,c}(q,\omega) &= (1 - U\Re e\ \Lambda^{aa}(q,\omega))\ U\ \Im m\ \Lambda^{bc}(q,\omega) - U^2\ \Im m\ \Lambda^{aa}(q,\omega)\ \Re e\ \Lambda^{bc}(q,\omega) \\
&\quad + U^2 \left[\Re e\ \Lambda^{ab}(q,\omega)\ \Im m\ \Lambda^{ac}(q,\omega)\ +\ \Im m\ \Lambda^{ab}(q,\omega)\ \Re e\ \Lambda^{ac}(q,\omega) \right]
\end{aligned}
\tag{67}
$$

7 Work in Progress: Constructing a Continuous Spectral Density $\Delta\rho(q,\omega)$ from the Moments $\Delta M_n(q)$

Since the continuous portion of the spectrum is bounded, we assume that $\Delta\rho(q,\omega)$ have the form:

$$
\Delta\rho(q,\omega) = \sum_{m=0}^{N} c_m(q)\ P_m(\omega/\omega_0(q)) \tag{68}
$$

where $c_m(q)$ are real constants and $P_m(x)$ are a set of orthogonal polynomials (we shall choose the Legendre polynomials) and $\omega_0(q)$ is the bound of the spectrum. The moments are defined as

$$
\Delta M_n(q) = \int_{-\omega_0}^{\omega_0} d\omega\ \omega^n\ \Delta\rho(q,\omega) \tag{69}
$$

which may be modified to either include or exclude the upper Hubbard band contributions. Then, the moments are represented by reduces to

$$
\Delta M_n(q) = \sum_{m} c_m(q) \int_{-\omega_0}^{\omega_0} d\omega\ \omega^n\ P_m(\omega/\omega_0) \tag{70}
$$

The coefficients $c_m(q)$ are determined the set of algebraic equations: reduces to

$$
\Delta M_n(q) = \sum_{m} c_m(q)\ \omega_0(q)^{n+1} \int_{-1}^{1} dx\ x^n\ P_m(x) \tag{71}
$$

The set of linear algebraic equations can be solved to yield the coefficients $c_m(q)$.

$$
\Delta M_n(q) = \sum_{m} c_m(q)\ \omega_0(q)^{n+1}\ I_{n,m} \tag{72}
$$

where

$$
I_{n,m} = \int_{-1}^{1} x^n\ P_m(x)\ dx \tag{73}
$$

The integrals are only non-zero for even $n+m$ due to parity. Using the recursion relation for the Legendre polynomials

$$xP_m(x) \;=\; \frac{(m+1)}{2m+1}P_{m+1}(x) + \frac{m}{2m+1}P_{m-1}(x) \tag{74}$$

and multiplying by x^{n-1} and integrating leads to:

$$I_{n,m} \;=\; \frac{(m+1)}{2m+1}I_{n-1,m+1} + \frac{m}{2m+1}I_{n-1,m-1} \tag{75}$$

These can be solved recursively, using $I_{0,0} = 2$, $I_{1,1} = \frac{2}{3}$ and are shown in the table. Thus, one needs to solve the set of equations

$$\Delta M_n(q) \;=\; \sum_m \; c_m(q)\; \omega_0(q)^{n+1}\; I_{n,m} \tag{76}$$

where the sum is restricted to either even values of m if n is even, or odd values of m if n is odd.

This method requires that the spectral density is continuous. Therefore, we remove the Dirac delta functions from the spectrum to produce a continuous spectrum $\delta\rho(q,\omega)$ given by

$$\Delta\rho(q,\omega) \;=\; \delta\rho(q,\omega) \;-\; 2\;\delta(\omega) \;+\; \sum_{i=1}^{3} \;\delta(\omega - \omega_i(q)) \tag{77}$$

where $\omega_i(q)$ are the energy eigenvalues of the peaks of the upper Hubbard bands. The moments of $\delta\rho(q,\omega)$ are expressed as

$$\delta M_n(q) \;=\; \Delta M_n(q) \;+\; \sum_{i=1}^{3} \;\omega_i(q)^n \tag{78}$$

for $n > 0$ and

$$\delta M_0(q) \;=\; -\,1 \tag{79}$$

for $n = 0$. The set of linear algebraic equations

$$\delta M_n(q) \;=\; \sum_m \; \delta C_m(q)\; \omega_0(q)^{n+1}\; I_{n,m} \tag{80}$$

can be solved to yield the coefficients $\delta C_m(q)$. The Legendre expansion for the continuous spectral density is given in terms of the coefficients by

$$\delta\rho(q,\omega) \;=\; \sum_{m=0}^{N} \;\delta C_m(q)\; P_m(\omega/\omega_0(q)) \tag{81}$$

Table 1: Non-zero values of $I_{n,m} = \int_{-1}^{1} x^n P_m(x)\, dx$ for $n \leq 5$

n	m	$I_{n,m}$
0	0	2
1	1	$\frac{2}{3}$
2	0	$\frac{2}{3}$
2	2	$\frac{4}{15}$
3	1	$\frac{2}{5}$
3	3	$\frac{4}{35}$
4	0	$\frac{2}{5}$
4	2	$\frac{8}{21}$
4	4	$\frac{16}{315}$
5	1	$\frac{2}{7}$
5	3	$\frac{8}{63}$
5	5	$\frac{16}{693}$

n	m	$I_{n,m}$
6	0	$\frac{2}{7}$
6	2	$\frac{12}{25}$
6	4	$\frac{32}{231}$
6	6	$\frac{32}{3003}$
7	1	$\frac{2}{9}$
7	3	$\frac{4}{15}$
7	5	$\frac{32}{429}$
7	7	$\frac{64}{6435}$

Table 2: Non-zero values of $I_{n,m} = \int_{-1}^{1} x^n P_m(x)\,dx$ for $n = 6$ and $n = 7$