Zero bias anomaly in the two-site Anderson-Hubbard model with Gaussian distribution for disorder

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Abstract. The Anderson-Hubbard model considers the correlation between disorder and other interactions in a strongly correlated electron system. Both disorder and correlations drive the metal-insulator transition but the densities of states behave in different ways. The zero bias anomaly (ZBA) referring to the V-dip shape of the density of states at the Fermi energy occurs in the strong disorder and strong interaction regime instead of a hard Coulomb gap in an insulator phase of strongly correlated interacting systems. In this paper, we use a Gaussian distribution for disorder to examine a two-site Anderson-Hubbard model. We also explain comprehensively the relationship between the phase diagram of ground states with various numbers of electrons and the behavior of the density of states. Furthermore, we want to investigate the effect of disorder distribution on the formation of the ZBA which originates from a hopping mechanism in two specific configurations.

1. Introduction

Metal-insulator transitions remain one of the most prominent issues in condensed matter physics. There are two main sources leading to the metal-insulator transition: electron correlations, for example on-site the Coulomb interaction prevailing in strongly correlated electron systems, and disorder which always exists in real materials. When the Coulomb interaction between on-site electrons becomes comparable with kinetic energy, electrons favor singly occupied states and thus the material undergoes a Mott-Hubbard metal-insulator phase transition at half-filling. In this case, a hard Coulomb gap separating a lower and an upper Hubbard band as described in the single-band Hubbard model \cite{1} opens at the Fermi energy $\epsilon_F$ in the density of states (DOS). Another way to bring about localization by impurity scattering in doped materials is disorder which causes an Anderson metal-insulator transition \cite{2}. Unlike the strongly correlated systems, the randomness of site energies induced by disorder localizes the wave function of conduction carriers characterized by the localization radius $R_{\text{loc}}$. The Anderson transition is normally realized by the divergence of the localization radius $R_{\text{loc}}$ when the system approaches a critical disorder.

The problem we address is how density of states at the Fermi energy (DOS($\epsilon_F$)) behaves if we treat both disorder and correlations on the same footing. Efros and Shklovskii (ES) \cite{3,4} showed that in the presence of long-range Coulomb interactions and disorder, the density of states close...
to the Fermi energy has a soft gap following a power-law scaling \( \text{DOS}(\epsilon) = |\epsilon - \epsilon_F|^{d-1} \), with \( d \) the spatial dimension. However, this law does not hold for the short-range interaction which plays a key role in many doped materials. Experimental results [5, 6, 7, 8, 9] have indicated that the density of states at the Fermi energy was essentially suppressed in some doped materials. However this phenomenon can not be explained by the ES theory.

The suppression of \( \text{DOS}(\epsilon_F) \) in the doped materials then emerges as an intriguing subject due to the lack of a fully comprehensive theory for disorder in correlated systems. A simplified model often used to describe the interplay of disorder and short-range Coulomb interaction is the Anderson-Hubbard model (AHM) for which the Hamiltonian is given by:

\[
H = -t \sum_{<ij>,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i \epsilon_i n_{i\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow},
\]

where electrons hop between nearest neighbor sites and \( n_{i\sigma} \) is the number operator for electrons with spin \( \sigma \) for site \( i \). The site energy \( \epsilon_i \) follows a distribution function \( P(\epsilon_i) \) where the disorder strength is characterized by a parameter \( \Delta \). The roles of electron interaction and disorder are represented by the on-site Coulomb energy \( U \) and the disorder strength \( \Delta \), respectively. A reasonably accurate phase diagram of the correlated metal, Mott-Hubbard insulator and correlated Anderson insulator phase can be established by dynamical mean field theory [10, 11, 12, 13]. Furthermore, other numerical calculations, such as exact diagonalization and quantum Monte Carlo simulations, surprisingly found the existence of a suppression of the DOS at the Fermi energy commonly known as the zero bias anomaly (ZBA), which depends intensively on doping \( \mu \), disorder strength \( \Delta \) and interaction strength \( U \) [14]. This soft gap has the width proportional to the hopping integral \( t \), which contradicts results for the energy scale achieved through other methods, \( U \) in the Hartree Fock approximation or \( t^2/U \) in the infinite \( U \) limit.

Recently a kinetic-driven ZBA was proposed in which the ZBA width depends only on the hopping integral \( t \) in the strongly disorder and strongly interaction regime [15, 16]. In order to confirm the key role of the hopping integral in the formation of ZBA, Atkinson’s group [17] exactly solved the molecular Anderson-Hubbard system and found that the hopping integral \( t \) lowered the ground-state energy by the linear combination of the lower and the upper Hubbard orbitals on neighboring sites. This kinetic-lowering mechanism is effectively worked in the strong disorder and strong correlation regime where a soft gap does appear with a width of \( \sqrt{2t} \). Their work concentrates mainly on the explanation of the origin of the ZBA with a uniform disorder distribution. Since a Gaussian distribution is more reasonable for real materials, in this paper we apply it for the two-site Anderson-Hubbard system to particularly investigate its effect on the ZBA formation.

2. Atomic limit

We can find the exact solution of the two-site Anderson-Hubbard model in the atomic limit \( t = 0 \), basing on the site eigen states \( |0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle \) corresponding to different electron numbers on each site where eigen energies are \( 0, \epsilon, \epsilon \) and \( 2\epsilon + U \), respectively. The ground state \( |\text{GS}\rangle \) depends on the Fermi level and is given by:

\[
|\text{GS}\rangle = \begin{cases} 
|0\rangle & \text{if } \mu < \epsilon_i, \\
|\uparrow\rangle, |\downarrow\rangle & \text{if } \mu - U < \epsilon_i < \mu, \\
|\uparrow\downarrow\rangle & \text{if } \epsilon_i < \mu - U.
\end{cases}
\]
From this, we can derive the retarded on-site Green’s function, which is:

\[ G(\omega) = \sum_{m,n,\sigma} \frac{|\langle n|c^\dagger_m|\Gamma\rangle|^2}{\omega + \mu - (E_0 - E_n) + i\delta} + \frac{|\langle m|c^\dagger_n|\Gamma\rangle|^2}{\omega + \mu + (E_0 - E_m) + i\delta}, \]

where \(|m\rangle \langle n|\) are excited states with energies \(E_m\) \((E_n)\) due to the process of creating (destroying) one electron in the ground state. For the simplicity of calculation, one can obtain the two-pole Green function of the \(i\)th site as:

\[ G(\epsilon_i, \omega) = \frac{\frac{1}{2} - \frac{\langle n_i \rangle}{2}}{\omega + \mu - \epsilon_i + i\delta} + \frac{\frac{\langle n_i \rangle}{2}}{\omega + \mu - \epsilon_i - U + i\delta}, \]

where \(\langle n_i \rangle = \langle c_i^\dagger c_i \rangle\). At half-filling, the Green function possesses an electron-hole symmetry with \(\mu = U/2\). Local density of states is given by:

\[ D(\epsilon, \omega) = -\frac{1}{\pi} \text{Im} G(\epsilon, \omega), \]

\[ = \left(1 - \frac{\langle n_i \rangle}{2}\right) \delta(\omega + \mu - \epsilon_i) + \frac{\langle n_i \rangle}{2} \delta(\omega + \mu - \epsilon_i - U). \]

In this work, we use a Gaussian distribution for the impurity which is

\[ P(\epsilon_i) = \frac{1}{\sqrt{2\pi} \Delta} \exp\left(-\frac{\epsilon_i^2}{2\Delta^2}\right), \]

with \(\Delta\) disorder parameter measuring disorder strength. Total density of states for the molecular system is then obtained as:

\[ D(\omega) = \int_{-\infty}^{\infty} P(\epsilon_i)D(\epsilon_i, \omega)d\epsilon_i, \]

\[ = D_1(\omega) + D_2(\omega), \]

where

\[ D_1(\omega) = \frac{1}{\sqrt{2\pi} \Delta} \left[e^{-\frac{(\omega - \mu)^2}{2\Delta^2}} \Theta(\mu - \omega) + e^{-\frac{\omega^2}{2\Delta^2}} \Theta(\omega - \mu)\right] \]

\[ D_2(\omega) = \frac{1}{2\sqrt{2\pi} \Delta} \left[e^{-\frac{(\omega - U)^2}{2\Delta^2}} \Theta(\mu - \omega) \Theta(\omega - \mu) + e^{-\frac{(\omega + \mu)^2}{2\Delta^2}} \Theta(\omega - \mu) \Theta(\mu + U - \omega)\right] \]

with \(\Theta(x)\) a Heaviside step function.

The normalized total density of states (DOS) analyzed in terms of partial densities of states \(D_1(\omega)\) and \(D_2(\omega)\) is illustrated in Fig. [1] with different disorder strengths. \(D_1(\omega)\) is the density of states obtained by zero-particle and two-particle ground state while \(D_2(\omega)\) is the density of states obtained by one-particle ground state. In the strong interaction case \((U = 12, t = 0)\), density of states mostly comes from the contribution of the one-particle ground state where following Eqs. [31-35], \(D_2(\omega)\) inherits two symmetrical separated peaks at \(\omega = \pm U/2\) corresponding to a lower-Hubbard orbital (LHO) and an upper-Hubbard orbital (UHO). In this case, the molecular system similarly behaves as the bulk system where the DOS shows a gap at the Fermi energy separating a lower Hubbard band and an upper Hubbard band for the insulator phase at half filling. The zero- and two- particle ground state contributes to the partial DOS \(D_1(\omega)\) which contains some spectral weight mainly around the Fermi energy. It is clearly seen that the increase of the disorder strength \((U = 12, \Delta = 4)\) enlarges the phase space following the condition (1).
Figure 1. Partial density of states $D_1(\omega)$, $D_2(\omega)$ and total density of states $D(\omega)$ of the molecular system with various disorder strengths $\Delta$ in the atomic limit. Fig. 1(a) and Fig. 1(b) show strong and weak interaction strength, respectively.

(see Fig. 2). Moreover, the extension of the zero or two electron ground state (see Fig. 2) also gives rise to the contribution of the spike at the Fermi energy presented in the partial density of states $D_1(\omega)$. The spectral weight enhancement of the spike with increasing disorder strength $\Delta$ has easily been observed from Eq. (8). As a result, the peaks at $\omega = \pm U/2$ of the spectral function $D_2(\omega)$ gradually broaden so that two peaks overlap and fill the gap at the Fermi level. We also notice that the disorder distribution strongly influences the shape of the DOS around the Fermi energy which presents a spike for the Gaussian distribution instead of a central plateau for the uniform distribution [15, 17]. Despite, disorder strength does not alter the shape of the spike at the Fermi energy.

If we go away from a picture of Mott physics to consider the disorder effect on the DOS
The dependence of ground states on site energies $\epsilon_1$, $\epsilon_2$ with different $U$ on-site interaction and $\Delta$ disorder strength in the atomic limit. The blocks with various colors of black, purple, brown, orange and yellow are correspondingly various ground states with zero, one, two, three and four electrons.

behavior, Fig. 1b will be an example for a weak interaction with different disorder strengths ($U = 2$). For $U$ rather small, $D_1(\omega)$ shows a great contribution to the spike peak at the Fermi energy compared with that of the large $U$ case while $D_2(\omega)$ shows a minor weight of two symmetrical peaks at $\omega = \pm U/2$. The redistribution of spectral weight with different on-site Coulomb interaction has also been observed in both bulk and molecular systems.

The dependence of the number of electrons of the ground states on site energies $\epsilon_1$, $\epsilon_2$ with different disorder strengths and with hopping term between two sites.

3. Effect of hopping term in the two-site systems

3.1. At half-filling $\mu = U/2$

Now we turn on the hopping term to investigate its effect on the phase space and on the density of states. Fig. 3 is plotted with the same parameters as in Fig. 2 except for $t = 1$. It is obviously
seen that the square shape of two-particle ground states is distorted especially around four
points symbolized by triangular and square points. The region of the two-particle ground state
around two triangular points $\epsilon_{1,2} = \epsilon_{2,1} + U = \pm \mu$ are enlarged toward the one-(three)
particle ground state region but this phenomenon is reversed around two square points. This distortion
around those points occurring for all cases of $U$ and $\Delta$ implies that the hopping mechanism
between two sites prefers two different configurations. The triangular points are referred to a
LHO-UHO arrangement where an upper Hubbard orbital (UHO) of one site is aligned with the
lower Hubbard orbital (LHO) of the other sites (see Fig. 4b ). In this situation, two electrons
can sit either on one site (double occupation) or on two different sites (single occupation). The
hopping term plays a key role in lowering the ground state energy of these two states by reducing
degeneracy of a singly occupied and a doubly occupied state (see Appendix for details), thus
the two-particle ground state is the lowest ground state of the system.

**Figure 4.** a) LHO-LHO configuration where two sites have same energies, $\epsilon_1 = \epsilon_2 = \pm \mu$ (square
points in Fig. 2); b) LHO-UHO configuration where the difference between two sites’ energy is
$U$, $\epsilon_{1,2} = \epsilon_{2,1} + U = \pm \mu$ (triangle points in Fig. 2).

**Figure 5.** Partial densities of states (a),(b) and total densities of states (c) of the molecular
systems with various $t$ values.
In the second configuration, square points ($\epsilon_1 = \epsilon_2 = \pm \mu$) refer to a LHO-LHO arrangement where a lower Hubbard orbital (LHO) of one site is aligned with the lower Hubbard orbital (LHO) of the other site (see Fig. 4a). In contrast to the first configuration, the one-(three) particle ground state have a chance to get more benefit from the disorder of site energies than the lowering of two-particle ground state due to hopping mechanism, thus the one-(three) particle ground state has the lowest energy in the competition of ground states if $U > 3t$ (see Appendix). It is clearly seen that in both cases, the hopping term only acts on the site energies close to the Fermi energy.

Figure 6. Total density of states of the molecular systems with various disorder strengths under the action of hopping term between two sites with strong interaction (a) and with weak interaction (b).

Figure 7. Total density of states of the molecular system with various on-site Coulomb interaction $U$ ($\Delta = 3; t = 1$).
one- and three-particle ground state and by the two-particle ground state, respectively. Since the contribution of the zero- and four-particle ground state for the density of states is almost negligible, we do not show it in the graph even though it is included in the total DOS $D(\omega)$. The increase of hopping energy does enlarge a soft gap around the Fermi energy in $D_1(\omega)$ whereas it insignificantly affects $D_2(\omega)$. The three (one)- particle ground state, which supports the configuration with LHO-LHO alignment of site’s energy close to $\mu$, contributes two poles around $\mu$. Following Eqs. [31-35] in the Appendix, one pole at $E^{(1+)}_t \approx \pm t$ corresponds to the transition from the one-particle ground state to the triplet states with its weight $z^{(1+)}_t = \frac{3}{2}$ while the other pole, $E^{(1+)}_\omega \approx \pm (t - \frac{3t^2}{U})$, excites (cancels) one electron from the ground state to the singlet state with its weight $z^{(1+)}_\omega$. When $t$ is fairly small ($t = 0.5$), these two poles are proportional to $t$, thus the linear dependence of the DOS around $\omega = 0$ would be observed due to the presence of sites with energies close to $\mu$. When $t$ is increased, $t^2/U$ is comparable with $t$, then a plateau near the Fermi energy is opened due to the constant weight $z^{(1+)}_t = \frac{3}{2}$ of the pole $E^{(1+)}_t$. For $D_2(\omega)$, the density of states at ZBA comes mostly from the two-particle ground state with the configuration of LHO-UHO alignment where poles of the two-electron Green function corresponds to the cancellation (creation) one electron on to the singlet ground state.

We also investigate the dependence of the ZBA on the various values of the on-site Coulomb interaction $U$ and of the disorder strengths $\Delta$. The width of this soft gap is mostly unbiased by the modification of $\Delta$ (see Fig. 6a) and of $U$ (see Fig. 7). Since these behaviors have been also observed in the uniform distribution [14], we can conclude that disorder distribution does not affect at all to the ZBA formation.

### 3.2. Away half-filling $\mu \neq U/2$

To investigate the behavior of the density of states away from half-filling $\mu \neq U/2$, results are shown in Fig. 8 (right) with the same parameters as above but at various values of chemical potential. We can obviously see the sudden reduction of the DOS at chemical potential which

![Figure 8](image-url)
also implies a change in the phase space around the chemical potential. The phase space diagram with \( \mu = U/4 \) (Fig. 8 (left)) is a typical example of the case away from half-filling. It is clearly seen that the action of the hopping term on those two configurations is the common feature not only at half filling but at any fillings as well. Since the hopping term reduces the degeneracy of the eigen states at the chemical potential, the DOS is abruptly decreased right at the chemical potential. It is worth to mention that this remarkable fact occurs only in the systems with strong disorder incorporated with strong correlated interactions where the presence of the chemical potential gives a great chance for the hopping term to show its key role in lowering the ground state energy even though it is rather weak compared with other energy scales.

4. Conclusions
In summary, the formation of V-shaped ZBA originates from the hopping term acting on the eigen states of the two-particle block to reduce the degeneracy. It is also noticed that although the hopping energy is much smaller than other interactions like \( U \) and \( \Delta \), it has a crucial contribution to the V-shaped dip in the density of states around the Fermi energy which is the unique phenomenon in the disordered systems. This effect is easily observed in the strongly correlated interacting case \( U \gg t \) where the presence of two-particle ground state prevails. We also examine the effect of the disorder strength and the on-site Coulomb interaction on the formation of the V-shaped dip. Even though the spectral weight of the density of states is redistributed with Coulomb interaction, the width of the ZBA is mostly unbiased by \( U \) and \( \Delta \). We also emphasize that disorder distribution does not affect to the origin and the V-shape of the ZBA.

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Appendix
Here we calculate the ground state and the Green function in each block with different numbers of electron in the two-site system. For the one-electron block, we define the one-electron basis states:

\[
c_{1,\sigma}^\dagger |0\rangle; \ c_{2,\sigma}^\dagger |0\rangle
\]

where \( c_{i,\sigma}^\dagger \) create one electron with spin \( \sigma \) on the \( i \)th site and the ket \( |0\rangle \) refers to the vacuum state without any electrons. The eigen energies can be derived by exact diagonalizing the matrix \( H_{mn}^{(1)} = \langle m^{(1)} | H | n^{(1)} \rangle \) with \( |m^{(1)}\rangle \)\( |n^{(1)}\rangle \) one electron basis states where

\[
H_{mn}^{(1)} = \begin{pmatrix}
\tilde{\epsilon}_1 & t \\
t & \tilde{\epsilon}_2
\end{pmatrix}
\]

Eigen energies are obtained by:

\[
E_{\pm}^{(1)} = \frac{\tilde{\epsilon}_1 + \tilde{\epsilon}_2 \pm \sqrt{\xi^2 + 4t^2}}{2}
\]

with \( \tilde{\epsilon}_1 = \epsilon_1 - \mu \), \( \tilde{\epsilon}_2 = \epsilon_2 - \mu \), \( \xi = \tilde{\epsilon}_1 - \tilde{\epsilon}_2 \) and the eigen states are correspondingly:

\[
|\psi_{\pm\sigma}^{(1)}\rangle = \alpha_{\pm}^{(1)} c_{1,\sigma}^\dagger |0\rangle + \beta_{\pm}^{(1)} c_{2,\sigma}^\dagger |0\rangle
\]

where

\[
\alpha_{\pm}^{(1)^2} = \frac{\sqrt{\xi^2 + 4t^2} \pm \xi}{2\sqrt{\xi^2 + 4t^2}}, \quad \beta_{\pm}^{(1)^2} = 1 - \alpha_{\pm}^{(1)^2}
\]
For the three-electron block, we follow the same procedure above, which gives

\[
H_{mn}^{(3)} = \begin{vmatrix}
2\tilde{\epsilon}_1 + \tilde{\epsilon}_2 + U & t & \\
t & \tilde{\epsilon}_1 + 2\tilde{\epsilon}_2 + U & \\
\end{vmatrix},
\]

\[
E_{\pm}^{(3)} = \frac{3(\tilde{\epsilon}_1 + \tilde{\epsilon}_2) + 2U \pm \sqrt{\xi^2 + 4t^2}}{2},
\]

and

\[
|\psi_{\pm}^{(3)}\rangle = \alpha_{\pm}^{(3)}|1_3\rangle + \beta_{\pm}^{(3)}|2_3\rangle.
\]

Here \(|0; 2\rangle = c_{21}^\dagger c_{21}^\dagger |0\rangle, |2; 0\rangle = c_{12}^\dagger c_{12}^\dagger |0\rangle,\)

\[
\alpha_{\pm}^{(3)} = \frac{\sqrt{\xi^2 + 4t^2} + \xi}{2\sqrt{\xi^2 + 4t^2}}, \quad \beta_{\pm}^{(3)} = 1 - \alpha_{\pm}^{(3)^2}
\]

For the two-electron block, we can separate into a triplet-state block where eigen states are

\[
|1_{(2)}^t\rangle = \frac{1}{\sqrt{2}} (c_{11}^\dagger c_{12}^\dagger + c_{12}^\dagger c_{11}^\dagger |0\rangle),
\]

\[
|2_{(2)}^t\rangle = c_{11}^\dagger c_{12}^\dagger |0\rangle,
\]

\[
|3_{(2)}^t\rangle = c_{12}^\dagger c_{11}^\dagger |0\rangle,
\]

with the same eigen energies \(E_{t}^{(2)} = \tilde{\epsilon}_1 + \tilde{\epsilon}_2\) and a singlet-state block where basis states are

\[
|1_{(2)}^s\rangle = \frac{1}{\sqrt{2}} (c_{11}^\dagger c_{21}^\dagger - c_{12}^\dagger c_{22}^\dagger |0\rangle),
\]

\[
|2_{(2)}^s\rangle = c_{11}^\dagger c_{21}^\dagger |0\rangle,
\]

\[
|3_{(2)}^s\rangle = c_{12}^\dagger c_{22}^\dagger |0\rangle,
\]

and the two-electron Hamiltonian is

\[
H_{mn}^{(2)} = \begin{vmatrix}
\tilde{\epsilon}_1 + \tilde{\epsilon}_2 & \sqrt{2}t & \sqrt{2}t \\
\sqrt{2}t & 2\tilde{\epsilon}_1 + U & 0 \\
\sqrt{2}t & 0 & 2\tilde{\epsilon}_2 + U \\
\end{vmatrix},
\]

Since the \(3 \times 3\) matrix can not be analytically solved, we find solution in two limiting cases. If \(\tilde{\epsilon}_1 \approx \tilde{\epsilon}_2,\)

\[
E_{s0}^{(2L)} = 2\tilde{\epsilon}_1 + U,
\]

\[
E_{s\pm}^{(2L)} = 2\tilde{\epsilon}_1 + \frac{U \pm \sqrt{U^2 + 16t^2}}{2}
\]

and

\[
|\psi_s^{(2L)}\rangle = \frac{1}{\sqrt{2}} (|2_{(2)}^s\rangle - |3_{(2)}^s\rangle),
\]

\[
|\psi_{s\pm}^{(2L)}\rangle = \alpha_{s\pm}^{(2L)}|1_{(2)}^s\rangle + \beta_{s\pm}^{(2L)}(|2_{(2)}^s\rangle + |3_{(2)}^s\rangle),
\]
where
\[
\alpha_{\pm}^{(2L)} = \sqrt{\frac{U^2 + 16t^2 \pm U}{2U^2 + 16t^2}},
\]
\[
\beta_{\pm}^{(2L)} = \frac{1}{2} (1 - \alpha_{\pm}^{(2L)})^2.
\]

If \( \tilde{\epsilon}_1 \approx \tilde{\epsilon}_2 + U \), neglect the basic state \(|2_{s}\rangle = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle\) with its higher energy, we obtain the two-electron eigen energies,
\[
E_{s\pm}^{(2U)} = \tilde{\epsilon}_1 + 3\tilde{\epsilon}_2 + U \pm \sqrt{4\eta^2 + 8t^2},
\]
and
\[
|\psi_{s\pm}^{(2)} \rangle = \alpha_{s\pm}^{(2)} |1_{s}\rangle + \tilde{\beta}_{s\pm}^{(2)} |3_{s}\rangle,
\]
where
\[
\alpha_{s\pm}^{(2)} = \frac{\sqrt{\eta^2 + 2t^2 \mp \eta}}{2\sqrt{\eta^2 + 2t^2}}, \quad \tilde{\beta}_{s\pm}^{(2)} = 1 - \alpha_{s\pm}^{(2)}^2
\]
with \( \eta = (U - \xi)/2 \).

In the LHO-LHO alignment \((\epsilon_1 = \epsilon_2 = \pm \mu)\), \( E_{s\pm}^{(2L)} \) is the ground state if \( U < 3t \). In the LHO-UHO alignment \((\epsilon_1 = \epsilon_2 \pm U = \mp \mu)\), \( E_{s\pm}^{(2U)} \) is always the ground state energy of the whole system with all values of \( U \) and \( t \).

For the chemical potential decides the position of the ground state, we can derive Green function corresponding to the ground state with different numbers of electron.

Now we calculate the Green function with different ground states if \( \tilde{\epsilon}_1 \approx \tilde{\epsilon}_2 + U \). For the one-electron ground state, the one-electron Green function is defined as:
\[
G_{\tilde{\epsilon}_1\tilde{\epsilon}_2}^{(1)}(\omega) = \sum_i \frac{z_i^{(1)+}}{\bar{\omega}^+ + \bar{E}_i^{(1)+}}
\]
where \( z_i^{(1)+} \) is the spectral weight of the pole at \( \bar{E}_i^{(1)+} \) and \( \bar{\omega}^+ = \omega - \mu + i\delta \). The spectral weights
and poles are obtained by

\[ z^{(1)+}_\pm = \frac{\alpha^{(2)}_\pm^2}{2} + \beta^{(1)}_\pm \beta^{(2)}_\pm + \sqrt{2} \alpha^{(1)}_- \alpha^{(2)}_+ \]
\[ = \frac{\alpha^{(2)}_\pm^2}{2} + \frac{1}{4} \left( \frac{\xi}{\sqrt{\xi^2 + 4t^2}} + \frac{\eta}{\sqrt{\eta^2 + 2t^2}} + \ldots \right) \]  
\[ (32) \]

\[ z^{(1)+}_t = \frac{|\langle \psi^{(2)}_s \mid c_{1\uparrow} \mid \psi^{(1)} \rangle|^2 + |\langle \psi^{(2)}_s \mid c_{2\uparrow} \mid \psi^{(1)} \rangle|^2}{2} + \frac{|\langle \psi^{(2)}_s \mid c_{1\downarrow} \mid \psi^{(1)} \rangle|^2 + |\langle \psi^{(2)}_s \mid c_{2\downarrow} \mid \psi^{(1)} \rangle|^2}{2} = \frac{\alpha^{(2)}_\pm^2}{2} + \frac{1}{4} \left( \frac{\xi}{\sqrt{\xi^2 + 4t^2}} + \frac{\eta}{\sqrt{\eta^2 + 2t^2}} + \ldots \right) \]  
\[ (33) \]

\[ \tilde{E}^{(1)+}_\pm = E^{(1)}_\pm - E^{(2)}_{s\pm} \]
\[ = -2\epsilon_2 - U - (\sqrt{\xi^2 + 4t^2} \pm \sqrt{\eta^2 + 2t^2}) \]  
\[ (34) \]

\[ \tilde{E}^{(1)+}_t = E^{(1)}_t - E^{(2)}_t \]
\[ = -\frac{\sqrt{\xi^2 + 4t^2}}{2} \]  
\[ (35) \]

For the three-electron ground state, the process to calculate the three-electron Green function is similarly carried out, which gives

\[ G_{\epsilon_1\epsilon_2}^{(3)}(\omega) = \sum_i \frac{z^{(3)-}_i}{\omega - \tilde{E}^{(3)-}_i}. \]  
\[ (36) \]

where

\[ z^{(3)-}_\pm = \frac{|\langle \psi^{(2)}_s \mid c_{1\downarrow} \mid \psi^{(3)} \rangle|^2 + |\langle \psi^{(2)}_s \mid c_{2\downarrow} \mid \psi^{(3)} \rangle|^2}{2} \]
\[ = \frac{\alpha^{(2)}_\pm^2}{2} + \beta^{(3)}_\pm \beta^{(2)}_\pm + \sqrt{2} \alpha^{(3)}_- \alpha^{(2)}_+ \]
\[ = \frac{\alpha^{(2)}_\pm^2}{2} + \frac{1}{4} \left( \frac{\xi}{\sqrt{\xi^2 + 4t^2}} + \frac{\eta}{\sqrt{\eta^2 + 2t^2}} + \ldots \right) \]  
\[ (37) \]

\[ z^{(3)-}_t = \frac{|\langle 1^{(2)}_t \mid c_{1\downarrow} \mid \psi^{(1)} \rangle|^2 + |\langle 1^{(2)}_t \mid c_{2\downarrow} \mid \psi^{(1)} \rangle|^2}{2} + \frac{|\langle 3^{(2)}_t \mid c_{1\downarrow} \mid \psi^{(1)} \rangle|^2 + |\langle 3^{(2)}_t \mid c_{2\downarrow} \mid \psi^{(1)} \rangle|^2}{2} = \frac{\beta^{(3)}_\pm^2}{2} + \frac{\alpha^{(3)}_\pm^2}{2} + \beta^{(3)-}_\pm^2 + \alpha^{(3)-}_\pm^2 \]
\[ (38) \]
\[ \tilde{E}_\pm^{(3)} = E^{(3)}_\pm - E^{(2)}_\mp \]
\[ = -2\tilde{e}_2 - U - \left( \sqrt{\xi^2 + 4t^2} \pm \sqrt{4\eta^2 + 8t^2} \right) \]
\[ = -\frac{\sqrt{\xi^2 + 4t^2}}{2} \]  
(39)
\[ \tilde{E}_t^{(3)} = E^{(3)}_t - E^{(2)}_t \]
\[ = -\frac{\sqrt{\xi^2 + 4t^2}}{2} \]  
(40)

For the two-electron ground state, the two-electron Green-function is:
\[ G_{\epsilon_1\epsilon_2}^{(2)}(\omega) = \sum_i \frac{z_i^{(2)+}}{\omega^+ + E_i^{(2)+}} + \frac{z_i^{(2)-}}{\omega^+ - E_i^{(2)-}} \]  
(41)

where
\[ z_i^{(2)+} = |\langle \psi^{(3)}_\pm | c_{1\uparrow} | \psi^{(2)}_s \rangle|^2 + |\langle \psi^{(3)}_\pm | c_{2\uparrow} | \psi^{(2)}_s \rangle|^2 - \]
\[ = (\alpha_\pm^{(3)} \beta^{(2)}_s + \beta_\pm^{(3)} \alpha^{(2)}_s + \sqrt{2})^2 + (\alpha_\pm^{(3)} \alpha^{(2)}_s / \sqrt{2})^2 \]  
(42)
\[ z_i^{(2)-} = |\langle \psi^{(1)}_\pm | c_{1\downarrow} | \psi^{(2)}_s \rangle|^2 + |\langle \psi^{(1)}_\pm | c_{2\downarrow} | \psi^{(2)}_s \rangle|^2 - \]
\[ = (\alpha_\pm^{(1)} \beta^{(2)}_s + \beta_\pm^{(1)} \alpha^{(2)}_s + \sqrt{2})^2 + (\alpha_\pm^{(1)} \alpha^{(2)}_s / \sqrt{2})^2 \]  
(43)
\[ \bar{E}_\pm^{(2)+} = E^{(2)}_\pm - E^{(3)}_\pm \]
\[ = -2\tilde{e}_1 - U - \left( \sqrt{4\eta^2 + 8t^2} \pm \sqrt{\xi^2 + 4t^2} \right) \]
\[ = -\frac{2\tilde{e}_1 - U - \sqrt{4\eta^2 + 8t^2} \pm \sqrt{\xi^2 + 4t^2}}{2} \]  
(44)
\[ \bar{E}_\pm^{(2)-} = E^{(2)}_\pm - E^{(1)}_\pm \]
\[ = 2\tilde{e}_2 + U - \left( \sqrt{4\eta^2 + 8t^2} \pm \sqrt{\xi^2 + 4t^2} \right) \]
\[ = -\frac{2\tilde{e}_2 + U - \sqrt{4\eta^2 + 8t^2} \pm \sqrt{\xi^2 + 4t^2}}{2} \]  
(45)

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