



Influence of screening effects and inter-site Coulomb repulsion on the insulating correlation gap

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Abstract

We study the effect of nearest neighbour Coulomb repulsion and of polarization screening on the conductivity gap in the Hubbard model at half filling. The gap is shown to be independent of the nearest neighbour Coulomb repulsion, but is effectively reduced by polarization screening.

The discovery of high temperature superconductivity has enhanced the interest in a set of Hubbard-like models that are used to describe the strongly correlated electronic structure of transition metal oxides. The parameters appearing in these models; hybridization, on-site and nearest neighbour Coulomb repulsion, are taken to be effective parameters [1–5]. The interaction between electrons is in principle slowly decaying with distance as $1/r$ but screening due to other electrons may drastically reduce the range of interaction, as discussed by Hubbard [5]. For a realistic description of materials, an effective on-site Coulomb repulsion U is used, rather than the unscreened atomic values U_0 . These effective parameters can be extracted from spectroscopic experiments. For the 3d transition metal Cu, for instance, the bare Coulomb repulsion $U_0 \approx 16$ eV is screened to $U \approx 4$ eV [6] and for C_{60} , $U_0 \approx 3.5$ eV is screened to a value of $U \approx 1.5$ eV [7].

In this paper we consider two long range effects which could reduce the effective value of U . One is

the nearest neighbour Coulomb interaction, the other occurs due to polarizability of surrounding atoms.

Consider the Hubbard model:

$$H_{\text{Hub}} = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U_0 \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$ and $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) an electron on site i with spin $\sigma = \uparrow$ or \downarrow . A nearest-neighbour pair is denoted by $\langle ij \rangle$. U_0 is the on-site Coulomb repulsion between two electrons on the same site. The hybridization between nearest-neighbour orbitals is denoted by t , allowing the particles to hop to adjacent sites. The on-site energies are taken to be zero.

The nearest neighbour Coulomb repulsion will effect the ground state energy if two neighbouring sites are both occupied:

$$H_{nn} = V \sum_{\substack{\langle ij \rangle \\ \sigma, \sigma'}} n_{i\sigma} n_{j\sigma'}, \quad (2)$$

V is the inter-site Coulomb repulsion between two electrons (holes) on neighboring sites. The Hamiltonian $H_{\text{Hub}} + H_{nn}$ is known as the extended Hubbard Hamiltonian [8–12]. We study the effect of small V on the conductivity gap. The motivation to study this is

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that recent papers suggest that V will reduce the effective value of U and therefore the gap in a half-filled system [13,14].

The conductivity gap, E_{gap} , is defined as the difference between the atomic ionization potential $E_I = E_{\text{GS}}^{N-1} - E_{\text{GS}}^N$ and the electron affinity $E_A = E_{\text{GS}}^N - E_{\text{GS}}^{N+1}$, where $E_{\text{GS}}^{N(\pm 1)}$ are the ground state energies of the $N(\pm 1)$ electron system. Here the conductivity gap is a direct measure of the effective on-site Coulomb repulsion. Exact diagonalization calculations of the conductivity gap in a two-dimensional extended Hubbard cluster show that E_{gap} is determined by U_0 and t only and is independent of V (see Fig. 2), contrary to what was asserted elsewhere [13].

This can easily be understood if one looks at the system in the localized limit ($t \rightarrow 0$): the average ground state energy per electron in the N -particle system, E_{GS}^N is $zV/2$, with z the number of nearest neighbours; $E_{\text{GS}}^{N+1} = E_{\text{GS}}^N + U + zV$ and $E_{\text{GS}}^{N-1} = E_{\text{GS}}^N - zV$. This results in a conductivity gap of U_0 . The calculations of the gap for finite t show that hybridization does not change this picture qualitatively. This also holds for a degenerate extended Hubbard model [15]. V therefore cannot be used to screen U_0 , as far as the E_{gap} is concerned.

Considering that the atoms are embedded in a polarizable surrounding, the effective Coulomb repulsion U is the energy required to move an electron from one atom to another, far away. In that case, U is equal to the difference of ionization potential E_I and electron affinity E_A of the solid. Removing an electron from a particular site, will polarize its surrounding, thereby lowering the ground state energy of the $N - 1$ electron system with an amount equal to the polarization energy E_{pol} , as schematically shown in Fig. 1.

In an ionic picture, the polarization or relaxation energy due to a point charge at site i is, within the dipole approximation, given [16] by

$$E_{\text{pol}} = \frac{1}{2} \sum_j \alpha_j F_j^2, \tag{3}$$

where j runs over all nearest-neighbours of i . It is assumed that the electric field due to the point charge at i is effectively screened to zero at lattice positions further away. The polarizability of an atom on site j is given by α_j and F_j is the electric field at site j . All atomic orbitals that are not explicitly included in the model Hamiltonian can in principle contribute to the polarizability.

This results in an extra term H_{pol} , in the Hamiltonian Eq. (1), which allows the atoms to polarize. The polarization term, assuming linear response, is defined as

$$H_{\text{pol}} = -P \sum_i \left(\sum_{j \in \{\text{n.n.}(i)\}} n_j \frac{\mathbf{R}_i - \mathbf{R}_j}{|\mathbf{R}_i - \mathbf{R}_j|} \right)^2 \tag{4}$$

where \mathbf{R}_i is the position vector of a given site i , $n_j = \sum_{\sigma} c_{j\sigma}^{\dagger} c_{j\sigma}$ and j runs over all nearest-neighbors of i . The sum over the nearest neighbours represents a quantity that is proportional to the electric field F_i on site i . As according to Eq. (3) the polarization energy is proportional to the electric field squared, the square appearing in Eq. (4) should be interpreted as the dot product of the (vectorial) electric field on site i .

For one electron in the polarizable lattice, the energy is given by $-E_{\text{pol}}$ and $E_{\text{pol}} = zP$, with z the coordination number. The state with two electrons far apart will have energy $-2zP = -2E_{\text{pol}}$, while the state with the two electrons on the same site has energy $U_0 - 4zP = U_0 - 4E_{\text{pol}}$. This because the polarization energy scales with the charge squared.

The Hamiltonian $H_{\text{Hub}} + H_{\text{pol}}$ is exactly diagonalized, using small clusters. In Fig. 2, the calculated value of the conduction gap E_{gap} is shown for a two-dimensional eight-site cluster at half-filling, as a function of the polarization energy parameter P . The inter-site hybridization is $t = 1$ eV and the bare on-site Coulomb repulsion $U_0 = 10$ eV. An increase in the polarizability yields a smaller gap. This implies that the effective Coulomb repulsion U decreases.

If we look at the system in the localized limit, there will be exactly one electron on each site. Therefore no microscopic electric field will be present that will polarize the surrounding atoms; the N -particle ground state energy E_{GS}^N is 0. Adding an electron will create one double occupied site and the energy of the $N + 1$ is raised by U_0 . The double occupancy will also result in polarization surrounding this double occupied site

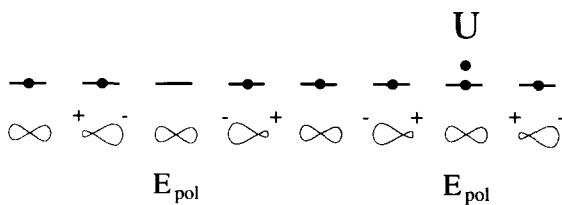


Fig. 1. Schematic representation of the excited states. A charge excitation will result in a polarization of the neighbouring atoms. The effective Coulomb repulsion U and induced polarizations are indicated.

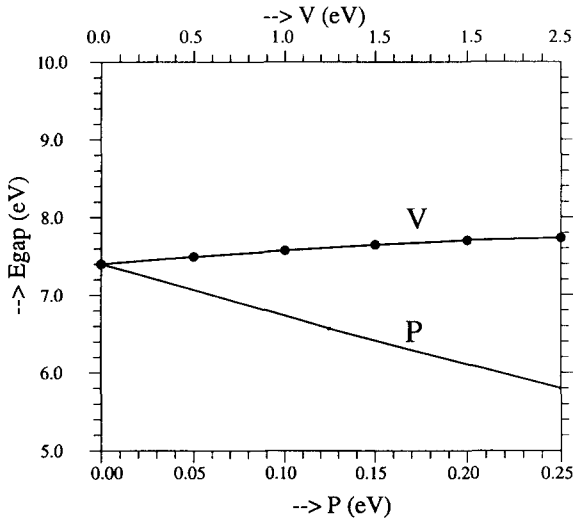


Fig. 2. Value of the conduction gap E_{gap} as a function of the inter-site Coulomb repulsion V and polarization screening P , for a two-dimensional eight-site extended Mott–Hubbard cluster. Upper curve with dots: V is varied between 0 and 2.5 eV. Lower curve: P is varied between 0 and 0.25 eV. The bare Coulomb repulsion U_0 is kept constant at 10 eV. The hybridization t is 1 eV.

and the energy lowering as a consequence of this polarization will be E_{pol} .

Therefore, we find that the electron affinity is increased with the polarization energy, yielding $E_A = E_{A0} + E_{\text{pol}}$. In the same way it is found that removing an electron from a particular site results in a lowering of the $N - 1$ electron ground state (see Fig. 1) because of E_{pol} . It yields therefore a decrease in the ionisation potential $E_I = E_{I0} - E_{\text{pol}}$. Here E_{I0} and E_{A0} denote the ionization potential and electron affinity when $E_{\text{pol}} = 0$. Now the effective Coulomb repulsion U is given by

$$U = U_0 - 2E_{\text{pol}}. \quad (5)$$

The calculations show that this argument also holds for finite values for the hybridization.

We conclude that our calculations show that the bare on-site Coulomb repulsion is not effectively reduced by a nearest neighbour interaction. The bare

on-site Coulomb repulsion is, however, effectively lowered by polarization screening effects. We argued that these effects can be understood qualitatively by examining the system in the localized limit.

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