THE EFFECT OF ELECTRON-ELECTRON INTERACTIONS
ON THE AVERAGE POLARIZABILITY OF A MESOSCOPIC
SYSTEM

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Abstract

A comparison between an analytical calculation of the polarizability of a
mesoscopic interacting system in the random phase approximation and numer-
ical exact diagonalization results is presented. While for weak interactions the
analytical calculation fits the numerical results rather well, deviations appear
for stronger interactions. This is the result of the appearance of intermediate
range correlations in the electron density, which suppresses the polarizability
below its classical value. The relevance to quantum dot systems is discussed.
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The study of the polarizability of small mesoscopic systems has a long history. Already in 1965 Gorkov and Eliashberg [1] have attempted to calculate the average polarizability of a small metallic grain by applying the concept of energy level repulsion from the random matrix theory (RMT) [2,3]. Their calculation, which can be backed by a non-linear sigma model calculation [4], shows that the average polarizability of a mesoscopic system \( \langle \alpha \rangle \propto (\kappa L)^{(d-1)} L^3 \) (here \( L \) is the length of the system and the inverse screening length \( \kappa^{(d-1)} = S_d e^2 N(0) \), where \( N(0) \) is the level density at the Fermi energy, \( S_d = 2\pi, (4\pi) \) for two (three) dimensional systems and \( \langle \ldots \rangle \) denotes an ensemble average). This result is much larger than the classical value of the polarizability \( \alpha \propto L^3 \). The reason for this apparent enhancement of the polarizability is, as pointed out by Strassler et. al. [5], the neglect of electron-electron (e-e) interactions which reduce the quantum corrections dramatically. Once \( \kappa L \gg 1 \), which for metallic systems corresponds to \( L \gg 1\text{Å} \), the polarizability is proportional to the volume [6]. The effect of e-e interactions in the random phase approximation (RPA) has been recently incorporated into the RMT formulation of the polarizability by Efetov [7]. The fluctuations in the grand-canonical ensemble were shown to be strongly suppressed by the e-e interactions [8,9], while the suppression is less significant in the canonical ensemble [10].

In recent experiments on disordered quantum-dots [11] it turned out that the ground-state energies of those dots show large fluctuations [12,13]. These fluctuations are larger than expected from RMT theory in which the e-e interactions are incorporated by the RPA [13]. This deviation from RMT theory is the result of the appearance of intermediate range correlations in the electron density as a result of strong e-e interactions. In this paper we shall show that the average polarizability is also affected by strong e-e interactions. While in the weak interaction regime the average polarizability is proportional to \( L^3 \), for strong interactions the polarizability tends to zero.

The polarizability may be written as

\[
\alpha = e^2 \frac{\partial}{\partial E} \int d\vec{r}(z - L/2)n(r)\Phi(r), \tag{1}
\]

where \( n(r) \) is the electronic density, \( \Phi(r) \) is the local electrostatic potential as a result of
applying an external electric field $E \hat{z}$ and the polarizability is calculated in the $\hat{z}$ direction. We shall begin by considering the weak interaction limit. In this limit one can treat both the disorder and the e-e interactions perturbatively. Taking into account the e-e interactions in the RPA one may rewrite Eq. (1) for the average polarizability as

$$\langle \alpha \rangle = e^2 N(0) \int d\vec{r} \, d\vec{r}' (z - L/2) \chi(\vec{r}, \vec{r}')(z' - L/2),$$

which after assuming a rectangular geometry and performing a Fourier transform results in

$$\langle \alpha \rangle = e^2 N(0) \left( \frac{L}{2} \right)^{2d} \sum_{\vec{q}} z(\vec{q})^2 \chi(\vec{q}),$$

where $\vec{q} = (n_x \pi/L)\hat{x} + (n_y \pi/L)\hat{y} + (n_z \pi/L)\hat{z}$ with $n_x, n_y, n_z = 0, 1, 2, \ldots$ (of course for 2D systems $\vec{q} = (n_x \pi/L)\hat{x} + (n_z \pi/L)\hat{z}$),

$$z(\vec{q}) = \frac{2}{L} \delta_{q_x=0} \delta_{q_y=0} \frac{(-1)^{(n_z+1)}}{q_z^2},$$

and

$$\chi(\vec{q}) = \left( \frac{2}{L} \right)^d \frac{1}{1 + N(0)\mathcal{V}U},$$

for short range interactions represented by an interaction potential $U(\vec{r}, \vec{r}') = \mathcal{V}U \delta(\vec{r} - \vec{r}')$ ($\mathcal{V} = a^d$ where $a$ is the range of the interaction and $d$ is the systems dimensionality). For the Coulomb interaction $U(\vec{r}, \vec{r}') = Ua/|\vec{r} - \vec{r}'|$, where $U$ is the strength of the Coulomb interaction between two particles at distance $a$, and

$$\chi(\vec{q}) = \left( \frac{2}{L} \right)^d \frac{q^{(d-1)}}{q^{(d-1)} + S_d N(0) a U}.$$ 

Inserting all the definitions in Eqs. (3-5) and performing the summation in Eq. (3) results, for short range interactions, in

$$\langle \alpha \rangle = \frac{2^d}{S_d 90} L^3 (\kappa L)^{(d-1)} \left( 1 + \frac{\mathcal{V}U}{L^d \Delta} \right)^{-1},$$

where $N(0) = (L^d \Delta)^{-1}$, and $\Delta$ is the single electron level spacing. For long range interactions

$$\langle \alpha \rangle = \frac{2^d}{S_d 90} L^3 (\kappa L)^{(d-1)} \sum_{n=1} \left( n^{(5-d)} \left( n^{(d-1)} + \frac{S_d a U}{\pi L \Delta} \right) \right)^{-1}.$$
Note that by using the constant $U$ to describe the strength of interactions between the electrons while using $e$ to describe the interaction between the electric field and the electrons we artificially create two different interaction scales. Nevertheless, this distinction is useful because it enables us to treat the interactions between the electrons by some appropriate effective interaction (say, short range interactions) while the interaction between the electric field and the electrons contributes a prefactor $(\kappa L)^{(d-1)}$ to the polarizability. Only in this sense can one understand the original treatment of Gorkov and Eliashberg [1] of the polarizability of non-interacting electrons. If we insert $U = e^2/a$ in Eq. (8) we obtain

$$\langle \alpha \rangle = \frac{2^d}{S_d 90} L^3 (\kappa L)^{(d-1)} \sum_{n=1}^{\kappa L / \pi} \left( n^{(5-d)} \left( n^{(d-1)} + (\kappa L / \pi)^{(d-1)} \right) \right)^{-1},$$

which for $\kappa L \gg 1$ gives the expected classical behavior

$$\langle \alpha \rangle \sim \frac{2^d \pi^{(d-1)}}{S_d 90} L^3.$$  

Thus the RPA approximation corresponds to the classical result $\alpha \propto L^3$.

In order to confirm the above results and to check their range of validity we have performed a numerical calculation of the polarizability for a system of interacting electrons on a 2D cylinder of circumference $L_x$ and height $L_z$. We used the following tight-binding Hamiltonian:

$$H = \sum_{k,j} (\epsilon_{k,j} + (j - (L_z + 1)/2) E) a_{k,j}^\dagger a_{k,j} - V \sum_{k,j} (a_{k,j+1}^\dagger a_{k,j} + a_{k+1,j}^\dagger a_{k,j} + h.c) + H_{int}$$

where $a_{k,j}^\dagger$ is the fermionic creation operator, $\epsilon_{k,j}$ is the energy of a site $(k, j)$, which is chosen randomly between $-W/2$ and $W/2$ with a uniform probability and $V$ is a constant hopping matrix element. We set the coupling the electrons and the external electric field $E$ to be unity (i.e., $e = 1$). $H_{int}$ is the interaction part of the Hamiltonian which for the short range interactions is given by:

$$H_{int} = U \sum_{\{k,j,l,p\}} a_{k,j}^\dagger a_{k,j} a_{l,p}^\dagger a_{l,p},$$

where $\{\ldots\}$ denotes the nearest-neighbor pairs of sites, and for the Coulomb interaction is equal to
\[ H_{\text{int}} = U \sum_{k,j \neq l,p} \frac{(a_{k,j}^\dagger a_{k,j} - K)(a_{l,p}^\dagger a_{l,p} - K)}{|\vec{r}_{k,j} - \vec{r}_{l,p}|/s}, \]  

(13)

where \( K \) is a positive background maintaining the charge neutrality and \( s \) is the lattice constant.

For a sample of \( M \) sites and \( N \) electrons, the number of eigenvectors spanning the many-body Hilbert space is \( m = \binom{M}{N} \). The many-body Hamiltonian may be represented by an \( m \times m \) matrix which is numerically diagonalized and the ground state eigenvector \( \Psi^E(k,j) \) is obtained for different values of the e-e interaction and electric field \( E \). Here we consider a \( 4 \times 4 \) lattice (i.e., \( M = 16 \) sites) and \( N = 4, 8 \) electrons. We chose \( W = 8V \) for which this system is in the metallic regime \(^1\) and average the results over 500 realizations for each value of interaction strength. The polarizability is calculated by

\[ \alpha = \frac{(d(E) - d(0))}{E}, \]  

(14)

where

\[ d(E) = \sum_{k,j} |\Psi^E(k,j)|^2(j - (L_z + 1)/2). \]  

(15)

Our main goal is to study whether the effect of the e-e interactions is predicted correctly by Eqs. (7-8). Therefore it is convenient to plot \( \langle \alpha(U = 0) \rangle / \langle \alpha(U) \rangle \) as function of interaction strength, which for short range interactions are is shown in Fig. 1. In order to evaluate Eq. (8) for the lattice case one should replace \( V/L^d \) by \( Z/(M - 1) \) where the average number of nearest neighbors, \( Z \), in our case is given by \( Z = 3.5 \) due to the presence of boundaries. The average level spacing is \( \Delta = 0.58V \) resulting in \( \langle \alpha(U = 0) \rangle / \langle \alpha(U) \rangle = 1 + 0.4U \) plotted in the figure. We can see a reasonable correspondence to the numerical values for both values of \( N \) for weak interactions, i.e., \( U < V \). For stronger values of interactions strong deviations appear for \( N = 8 \), while for \( N = 4 \) the correspondence holds. We shall discuss the reason for this behavior shortly.

For the long range interactions the results are shown in Fig. 2. For a lattice system one should replace \( S_2 = L^{-1} \int d^2r/r = 2\pi \) in Eq. (8) by \( S_2^* = L^{-1} \sum_{k,j \neq l,p} |\vec{r}_{k,j} - \vec{r}_{l,p}|^{-1} \).
which in our case results in \( S_2^* = 2.44 \). Thus, after incorporating \( S_2^* \) in Eq. (8) one obtains \( \langle \alpha(U = 0) / \langle \alpha(U) \rangle = 1 + 0.32U \) plotted in the figure. Again a good agreement between the theory and the numerical results is seen for weak interactions \( (U < 4V) \), while deviations appear for both values of \( N \) for strong interactions.

Thus, the RPA describes the polarizability rather well as long as the interactions are not too strong, resulting in the classical polarizability of Eq. (10) \( \alpha \propto L^3 \). Once the interactions are strong the polarizability is suppressed compared to the classical value, i.e., \( \alpha \ll L^3 \).

The reason for the deviations is the appearance of intermediate range correlations for strong interactions. This may be clearly seen by defining a two point correlation function:

\[
C(r) = \frac{\sum_{k,j>l,p} C(\vec{r}_{k,j} - \vec{r}_{l,p}) \delta_{\vec{r}_{k,j} - \vec{r}_{l,p},r}}{\sum_{k,j>l,p} \delta_{\vec{r}_{k,j} - \vec{r}_{l,p},r}},
\]

where

\[
C(\vec{r}_{k,j} - \vec{r}_{l,p}) = \left\langle \frac{[|\Psi(k,j)|^2 - \langle |\Psi(k,j)|^2 \rangle][|\Psi(l,p)|^2 - \langle |\Psi(l,p)|^2 \rangle]}{\langle |\Psi(k,j)|^2 \rangle \langle |\Psi(l,p)|^2 \rangle} \right\rangle.
\]

In Fig. 3 we present the correlation \( C(r = \sqrt{5}s) \) for different values of interaction. Under the RMT assumptions, as well as for RPA, we expect \( C(r = \sqrt{5}s) \to 0 \). On the other hand, once Wigner crystallization occurs we expect \( C(r = \sqrt{5}s) \to -1 \) for \( N = 8 \), while \( C(r = \sqrt{5}s) \to 1 \) for \( N = 4 \). It can be clearly seen that for weak interactions (i.e., \( U < V \) for short range interactions and \( U < 4V \) for Coulomb interactions) \( C(r = \sqrt{5}s) \sim 0 \). For stronger interactions a transition towards the Wigner crystal values of \( C(r = \sqrt{5}s) \) is clearly seen for both the Coulomb and the short range interactions in the half filled case \( (N = 8) \).

This correlation is a sign of the appearance of intermediate range order in the electronic system. We call this intermediate range order and not long range order since it decreases on the order of several lattice sites. Only for stronger interactions does a real, long ranged, Wigner crystal appear. Naturally, for lower fillings \( (N = 4) \) the transition is much weaker for the Coulomb interactions and absent for short range interactions.

This behavior is the explanation for the deviations from the perturbative results of the polarizability at strong interactions seen in Figs. 2. As long as there is no intermediate range order, RPA holds. Once intermediate range order appears, the electrons are
correlated, i.e., the electrons have a spatial order and exhibit a strong resistance to being compressed. Therefore, the application of an external electric field has less influence on their spatial distribution and \( \langle \alpha(U >> V) \rangle \rightarrow 0 \) resulting in the strong deviation of \( \langle \alpha(U = 0) \rangle / \langle \alpha(U >> V) \rangle \) from the linear dependence especially for the half-filled cases in which the effect of intermediate range order is the largest. For \( N = 4 \) the deviations towards larger values of \( \langle \alpha(U = 0) \rangle / \langle \alpha(U >> V) \rangle \) are weaker for the Coulomb interactions since the spatial correlations are smaller and do not appear for the short range interactions where no correlations exist.

In order to consider the relevance of the above results to an experimental situation one must determine the ration \( U/V \). For quantum dots \( U/V > 3 \) is realized, and strong evidence of the intermediate range order appears in the behavior of the ground state energy fluctuations [13]. Therefore, one might expect that these systems will show a strong decrease in their polarizability beyond the classical value due to the appearance of intermediate range order.

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FIG. 1. The ratio $\langle \alpha(U = 0) \rangle / \langle \alpha(U) \rangle$ for short range interactions. The numerical results for $N = 8$ are represented by circles and for $N = 4$ by squares. The weak interaction regime is plotted in (a), while in (b) a larger range of interactions is presented.
FIG. 2. The same as in Fig. 1 for the Coulomb interactions.
FIG. 3. The two point correlation $C(r = \sqrt{3}s)$ for (a) short range interactions, (b) long range interactions. Circles correspond to $N = 8$ and squares to $N = 4$. 