Static overscreening and nonlinear response in the Hubbard Model

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We investigate the static charge response for the Hubbard model. Using the Slave-Boson method in the saddle-point approximation we calculate the charge susceptibility. We find that RPA works quite well close to half-filling, breaking, of course, down close to the Mott transition. Away from half filling RPA is much less reliable: Already for very small values of the Hubbard interaction \( U \), the linear response becomes much more efficient than RPA, eventually leading to overscreening already around quite moderate values of \( U \). To understand this behavior we give a simple argument, which implies that the response to an external perturbation at large \( U \) should actually be strongly non-linear. This prediction is confirmed by the results of exact diagonalization.

I. INTRODUCTION

Motivated by the surprising accuracy of the random phase approximation (RPA) for a half-filled, generalized Hubbard model with orbital degeneracy, we ask how well RPA reproduces the screening in correlated systems in general. While it properly describes the screening when the kinetic energy is much larger than the interaction energy, RPA becomes wrong in the opposite limit. Its main deficiency is that it completely misses the break-down of the screening at the Mott transition. Nevertheless, as the quantum Monte Carlo calculations in Ref. 1 have shown, RPA gives a surprisingly accurate description of the static charge response on the metallic side of the Mott transition, until the system is quite close to the transition point. Away from half filling (or, more generally, integer filling) one would expect the system to become more metallic, and hence, RPA to work even better. We will see, however, that this not the case.

In the present study we use a Slave-Boson method to calculate the linear charge response. The advantage over more elaborate methods like quantum Monte Carlo (QMC) or exact diagonalization are (i) the possibility to treat very large systems, such that finite size effects become negligible, (ii) the efficiency of the method, which allows us to thoroughly study the whole parameter space of different densities and interactions, and (iii) the possibility to directly calculate the linear response, which in Lanczos or QMC calculations has to be extrapolated from several calculations for different perturbations of finite strength.

There have been already a number of works determining the linear response from a one-loop expansion around the Slave-Boson saddle-point solution, but they mainly focused on the structure factors and the spin response. In contrast, here we are interested in the static density response, which can be calculated at the saddle-point level, avoiding the problems encountered when considering Gaussian fluctuations of the Slave Bosons. In that sense our approach is related to that of Refs. 13 and 14, with the main difference that we consider the linearized saddle-point equations, in order to directly obtain the linear response. As for the accuracy of the results, based on the experience of previous works, we expect that the static response should be well described.

The model we consider here is the one-band Hubbard model with nearest and next-nearest neighbor hopping on a square lattice. It is introduced in Sec. II.A. We are in particular interested in the response to a point charge. In Sec. II.B we describe the approach for calculating the charge response using Slave-Bosons at the saddle-point level. To check the method and its accuracy, we compare with the result of exact diagonalization. In Sec. II.C we give the results of our calculations: the screening as a function of filling and interaction. The most striking result is that, already for quite moderate interaction, the systems shows a response that is stronger than the perturbation (overscreening). The response, of course, strongly depends on the doping and changes with the next-nearest neighbor hopping, being enhanced close to the van Hove singularity. Comparing with the random phase approximation, we find that, contrary to our expectation, RPA works best close to half filling. In Sec. III we give an interpretation of these results. Both, doping dependence and overscreening can be understood using simple large-\( U \) arguments. We also discuss why, by the same arguments, we do not obtain overscreening in the RPA and that overscreening does not mean that the systems becomes unstable. The argument for explaining the overscreening does, however, imply that the charge response of the non-half-filled Hubbard model should be strongly nonlinear, which we numerically confirm using exact diagonalization. Indeed, we find that the stronger the response, the more nonlinear it will be. A conclusion, Sec. IV, closes the presentation.

We finally would like to point out that overscreening in the Hubbard model has been observed before and a proof, although in quite a different spirit from ours, for the necessity of overscreening for large interactions has been given.
II. SLAVE-BOSON CALCULATIONS

A. Model

We consider the one-band Hubbard model with nearest and next-nearest neighbor hopping \((t, t')\), respectively,
\[
H = -t \sum_{\langle i,j \rangle, \sigma} f_{j,\sigma}^\dagger f_{i,\sigma} - t' \sum_{\langle i,j \rangle, \sigma} f_{j,\sigma}^\dagger f_{i,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}
\]
on a square lattice with lattice constant \(a\). For the non-interacting system \((U = 0)\) the dispersion relation is
\[
\varepsilon_k = -2t(\cos(k_x a) + \cos(k_y a)) - 4t' \cos(k_x a) \cos(k_y a)
\]
and the density of states has a logarithmic van Hove singularity at \(4t'\).

We ask for the response to the perturbation by an external point charge \(c\) at site \(r_c\), corresponding to an extra term \(cU \sum \delta n_c\) in the Hamiltonian. Expanding the external potential in plane waves, we find, given the static susceptibility \(\chi_q\) for wave vector \(q\), for the induced charge at site \(r_i\)
\[
\delta n_i = \sum_{q \neq 0} \chi_q \delta V_q = \frac{cU}{N} \sum_{q \neq 0} \chi_q e^{iq(r_i-r_c)},
\]
where we have excluded the \(q = 0\) component, since we are really interested in the response for a system with fixed number of electrons. Below we will particularly focus on the response at the site with the point charge \(\Delta n = \delta n_{i=0}\).

For the noninteracting system the susceptibility (per spin) \(\chi_q^{(0)}\) is given by (we give a more general definition, which we will need below)
\[
\chi_q^{(0)} = \frac{1}{N} \sum_k \frac{\varepsilon_k f_k - \varepsilon_{k+q} f_{k+q}}{\varepsilon_k - \varepsilon_{k+q}}
\]
(2)

We now give a brief outline of the linearization procedure. We start from the Kotliar-Ruckenstein formulation of the Slave-Boson method.\(^8\) It maps the physical Fermions onto composite particles of pseudofermions and four Bosons, representing empty \((e_i)\), singly \((p_{i,\sigma})\), and doubly \((d_i)\) occupied sites. Constraints, ensuring consistency between pseudofermions and Bosons, enforced by Lagrange parameters \((\lambda_i^{(1)}\) and \(\lambda_i^{(2)}\), are introduced to eliminate the unphysical states in the enlarged Hilbert space. In this enlarged space, the Hamiltonian can be represented in a form, having kinetic terms with mixed fermionic-bosonic character (renormalized hopping), while the interaction becomes purely bosonic and bilinear. The pseudofermions, merely occurring in bilinear terms, can then be integrated out exactly, and one is left with a purely bosonic action integral (including the Lagrange parameters that ensure the coupling to the pseudofermions). The simplest approach to the bosonic action integral is the saddle-point approximation, in which all Bose fields are time independent. The Slave-Boson action then takes the form
\[
\int_0^\beta d\tau S(\tau) = \sum_i \left[ \lambda_i^{(1)} e_i^2 + \sum_\sigma \left( \lambda_i^{(1)} - \lambda_i^{(2)} \right) (p_{i,\sigma})^2 + \left( U + \lambda_i^{(1)} - \sum_\sigma \lambda_i^{(2)} \right) d_i^2 - \lambda_i^{(1)} \right] - \sum_{i,\sigma} \ln \left[ 1 + e^{-\beta \varepsilon_{i,\sigma}} \right]
\]
where
\[
z_{i,\sigma} = \frac{e_{i,\sigma} + p_{i-\sigma}d_i}{\sqrt{1 - d_i^2} \sqrt{1 - e_{i,\sigma}^2}}
\]
for \(n = 0\). Here \(N\) is the number of lattice sites, the sum is over all states (first Brillouin zone), and \(f_k = (1 + \exp(-\beta(\varepsilon_k - \mu)))^{-1}\) is the Fermi-Dirac function. In case of degeneracy the quotient in (2) becomes the differential. In RPA the susceptibility is
\[
\chi_q^{RPA} = \frac{2\chi_q^{(0)}}{1 - 2U\chi_q^{(0)}}.
\]

B. Method

As an efficient way for calculating the static response we choose the Slave-Boson method, which will allow us to easily explore the parameter space (fillings \(n_\sigma\), interactions \(U\), hoppings \(t'\)) for quite big lattices (100 \times 100) and low temperatures \((\beta = 100/t)\). We use the formalism developed by Kotliar and Ruckenstein\(^9\) (since we are only interested in the density response of the paramagnet, we need not explicitly take care of the spin-rotation invariance).\(^9\) Instead of studying Gaussian fluctuations of the Slave-Boson action around the saddle-point (one-loop expansion\(^9\)), we stay at the mean-field level, simply linearizing the saddle-point equations for the perturbed system. In that sense, our approach is closer to that of Refs.\(^3\) and \(^4\) where the full saddle-point equations for a system with finite perturbation were solved. We thus avoid the problems related to the representation of the hopping operator.\(^4\)\(^5\) The main advantage of our linearized saddle-point equations is, that for a plane-wave perturbation the resulting linear system becomes block diagonal, with identical blocks of size 5 \times 5, independent of system size. We expect our method to give a good description of the true screening, given the good experience, in particular for static quantities.\(^3\)\(^4\)\(^5\)
and the $\varepsilon_{n,\sigma}$ are the eigenvalues of the renormalized Hamiltonian

$$H_\sigma = -\sum t_{i,j} z_{i,\sigma} z_{j,\sigma} f_{j,\sigma} f_{i,\sigma} + \sum_i \left( \lambda_i^{(2)} - \mu + V_i \right) n_i. \quad (3)$$

The mean-field values of the bosons and the Lagrange parameters are determined from the saddle-point equations

$$0 = \beta^{-1} \frac{\partial S}{\partial \varepsilon_i} = 2 \lambda_i^{(1)} - \varepsilon_i + \sum_{n,\sigma'} \frac{1}{1 + e^{-\beta \varepsilon_{n,\sigma'}}} \frac{\partial \varepsilon_{n,\sigma'}}{\partial \varepsilon_i},$$

$$0 = \beta^{-1} \frac{\partial S}{\partial \varepsilon_{p,\sigma}} = 2 \left( \lambda_i^{(1)} - \lambda_i^{(2)} \right) p_{i,\sigma} + \sum_{n,\sigma'} \frac{1}{1 + e^{-\beta \varepsilon_{n,\sigma'}}} \frac{\partial \varepsilon_{n,\sigma'}}{\partial \varepsilon_{p,\sigma}},$$

$$0 = \beta^{-1} \frac{\partial S}{\partial d_i} = 2 \left( U + \lambda_i^{(1)} - \sum_{\sigma} \lambda_i^{(2)} \right) d_i + \sum_{n,\sigma'} \frac{1}{1 + e^{-\beta \varepsilon_{n,\sigma'}}} \frac{\partial \varepsilon_{n,\sigma'}}{\partial d_i},$$

$$0 = \beta^{-1} \frac{\partial S}{\partial \lambda_i^{(1)}} = \varepsilon_i^2 + \sum_{\sigma} p_{i,\sigma}^2 + d_i^2 - 1,$$

$$0 = \beta^{-1} \frac{\partial S}{\partial \lambda_i^{(2)}} = -\varepsilon_i^2 - d_i^2 + \sum_{n,\sigma'} \frac{1}{1 + e^{-\beta \varepsilon_{n,\sigma'}}} \frac{\partial \varepsilon_{n,\sigma'}}{\partial \lambda_i^{(2)}}.$$

For finite temperature $\beta$, this nonlinear system of equations has to be solved self-consistently, since the eigenvalues $\varepsilon_{n,\sigma}$ of the renormalized Hamiltonian (3) depend on the mean-field values of the bosonic fields. The Fermionic terms are most easily evaluated in the form

$$\sum_{n,\sigma'} f(\varepsilon_{n,\sigma'}) \frac{\partial \varepsilon_{n,\sigma'}}{\partial x_{\sigma}} = -\frac{1}{\pi} \Im \int_{-\infty}^{\infty} d\epsilon \ f(\epsilon) \ Tr \left( G_{\sigma'}(\epsilon) \frac{\partial H_\sigma}{\partial x_{\sigma}} \right),$$

where $G_{\sigma}(\epsilon) = (\epsilon - H_\sigma)^{-1}$ is the Greens function. For the homogeneous system, the Boson variables are independent of the site index, and solving the saddle point equations for the magnetron ($p \equiv p_\uparrow = p_\downarrow$) essentially reduces to self-consistently solving a 3rd-order polynomial in $d^2$.

For calculating the linear response, it is easiest to consider external potentials $V_i = \delta V_q \cos(q r_i)$, which give rise to a response: $n_i = n + \delta n \cos(q r_i)$ and $\varepsilon_i^2 = \varepsilon_i^2 + 2\delta \varepsilon \cos(q r_i)$. Expanding to first order and using the relation

$$-\frac{1}{\pi} \Im \int_{-\infty}^{\infty} d\epsilon \ f(\epsilon) \ \delta n n \sum G_{i,j}(\epsilon) \cos(q r_j) G_{j,i}(\epsilon) = \chi^{SBMF,n}_{\epsilon}(q) \cos(q r_i),$$

where $\chi^{SBMF,n}_{\epsilon}(q)$ is calculated as (3), but using the eigenvalues of the renormalized Hamiltonian (3) for the homogeneous solution. We can factor out the coordinate dependence; i.e., we find that the linearized the saddle-point equations are block diagonal, with identical $5 \times 5$ blocks of the form

$$\begin{pmatrix}
A_{zz} z_c + D(z_{ce} - \frac{\varepsilon}{e}) & A_{zz} z_p + D z_{cp} & A_{zz} z_d + D z_{cd} & e & B z_c \\
A_{zp} z_c + D z_{pc} & A_{zp} z_p + D(z_{pp} - \frac{\varepsilon}{p}) & A_{zp} z_d + D z_{pd} & 2p & B z_p - 2p \\
A_{zd} z_c + D z_{dc} & A_{zd} z_p + D z_{dp} & A_{zd} z_d + D(z_{dd} - \frac{\varepsilon}{d}) & d & B z_d - 2d \\
e & 2p & d & 0 & 0 \\
B z_c & B z_p - 2p & B z_d - 2d & 0 & C
\end{pmatrix} = \begin{pmatrix}
de/dV_q & dp/dV_q & dd/dV_q & -B z_c & -B z_p \\
-B z_c & -B z_p & -B z_d & 0 & -C
\end{pmatrix}$$

Here the $z_c$, $z_{ce}$, $z_{pd}$ denote the partial derivatives of $z$, and, since we have set $p = p_\sigma$ (paramagnetic solution), the partial derivative with respect to $p$ means the sum of the partial derivatives with respect to $p_\uparrow$ and $p_\downarrow$. Also, we have introduced $A = 4\chi^{(0,2)}_q - 6\varepsilon_0$, $B = 2(\chi^{(0,1)}_q - n_\sigma)/z$, $C = \chi^{(0,0)}_q / z^2$, and $D = 2z\varepsilon_0$, where $\varepsilon_0$ is the energy density per spin and the $\chi^{(0,n)}_q$ the susceptibilities (3) for the noninteracting part of the unrenormalized Hamiltonian taken at the renormalized temperature $z^2\beta$ and Fermi energy $\mu - \lambda^{(2)}_i / z^2$. Solving the linear system, the susceptibility is given by $\chi^{SBMF}_q = \partial n_q / \partial V_q = 4(p dp/dV_q + d dd/dV_q)$, and the response to a point charge follows from eqn. (1).

To check the method, and to verify our code, we compare the results of the Slave-Boson calculation to the linear response calculated by exact diagonalization for a $4 \times 4$ Hubbard model. As can be seen from Fig. 4, the Slave-Boson results basically reproduce the response, although they tend to slightly underestimate the screening.
The good agreement does not come as a surprise. The important conclusion to draw from the asymptotic expansion is that for large $U$, to leading order, the susceptibility is independent of the interaction. Therefore, as long as the large-$U$ value does not happen to vanish (as is the case for $n_\sigma = 0, 1/2, 1$), the linear response to a point charge $dn/dc$ will, to leading order, grow linearly with $U$ — beyond any limit.

C. Results

1. Overscreening

The results of the Slave-Boson mean-field calculations for the response to a point charge as a function of filling $n_\sigma$ and interaction $U$ for different hoppings $t'$ are shown in Figure 1. The most striking feature is that only exactly at half-filling, the response vanishes (at the Mott transition), while for any other filling $n_\sigma \neq 1/2$ the induced charge density on the site with the test charge eventually increases linearly with $U$. The reason is that, in the limit of $U$ going to infinity, the susceptibility of the non-half-filled system stays finite, only for $n_\sigma = 1/2$ does $\chi_q$ vanish (see Fig. 3). This necessarily means that for strong enough interaction and $n_\sigma \neq 1/2$ the induced charge will be larger than the perturbation. What is quite surprising is, that this overscreening already sets in for very moderate values of $U$. As a function of the next-nearest neighbor hopping, we find overscreening for (see the first contour line in Fig. 3):

$$t'/t \sim \frac{U/t}{6 5 4 3 2}$$

We also remark that, according to the comparison with the exact results for a small system (Fig. 3), the Slave-Boson results might even somewhat underestimate the true response.

The second striking feature is the strong doping dependence of the response. It tends to be strongest for quarter filling $(n_\sigma = 1/4$ or $3/4$), while it vanishes when approaching the Mott- or band-insulating regions. This doping dependence is somewhat modified by the next-neighbor hopping $t'$: The screening becomes enhanced in the neighborhood of the van Hove singularity (at $4t'$). For $t'/t = -1/2$, where the van Hove singularity is at the lower band-edge, this enhancement is particularly pronounced, while for $t' = 0$, where the singularity is at half filling, it is masked by the Mott transition. We note that around half filling the system could become antiferromagnetic and that close to the van Hove singularity and for large $U$ there could be ferromagnetism, while in our calculations we always restrict ourselves to the paramagnetic state.
FIG. 2. Linear response to the perturbation by a point charge in the Hubbard model as a function of filling $n_\sigma$ and interaction $U$ for different values of the next-nearest neighbor hopping matrix element $t'$. The calculations use the Slave-Boson method in the mean field approximation and were performed for square lattices of size $100 \times 100$ at $\beta = 100/t$. $dn$ is the electron density that is induced on a site with an infinitesimal test-charge $dc$, i.e. on a site with external potential $dc U$. Contour lines are drawn for $-dn/dc = 1, 1.5, 2, \ldots$, i.e. the first contour line marks the onset of overscreening. It is clear that, as the van Hove singularity (at $4t'$) is shifted to lower energies, the response for less than half filling gets increasingly stronger. For $t' = 0$ the singularity is at half filling and moves towards smaller $n_\sigma$, until it reaches the lower band-edge for $t'/t = -1/2$. 

$100 \times 100$ lattice, $\beta t = 100$, $t'/t = 0.00$

$100 \times 100$ lattice, $\beta t = 100$, $t'/t = -0.10$

$100 \times 100$ lattice, $\beta t = 100$, $t'/t = -0.20$

$100 \times 100$ lattice, $\beta t = 100$, $t'/t = -0.30$

$100 \times 100$ lattice, $\beta t = 100$, $t'/t = -0.40$

$100 \times 100$ lattice, $\beta t = 100$, $t'/t = -0.50$
2. Comparison with RPA

The overscreening obviously has important implications for the validity of the RPA. Since in the RPA the response can at most equal the perturbation (perfect screening), it clearly will not work well, wherever there is overscreening. From the direct comparison in Fig. 3 we find, however, that it already starts to fail for much smaller values of $U$. (The calculations are for a Hubbard model with non-zero next-nearest neighbor hopping, to avoid perfect nesting.) Surprisingly, RPA seems to work best close to half filling, but, of course, only well below the Mott transition. Note that the contour lines around $n_\sigma = 1/2$ in Fig. 3 first mark increasing values, but, when approaching the Mott transition, turn negative (see also Fig. 5). When going away from half filling, where one expects the correlated system to become more metallic, RPA rapidly fails to give a good description of the screening. For better visualization, we give a direct comparison of RPA and the result of the Slave-Boson calculation in the two regimes (close to and far from half filling) in figure 5. For half-filling, RPA only somewhat underestimates the response for small $U$, but fails to describe the eventual break-down of the screening at the Mott transition. Overall, for $n_\sigma = 1/2$ the error in $dn/dc$ is $\lesssim 0.15$ (relative error $\lesssim 20\%$) up to $U$ larger than $U_c/2$. This is consistent with what was found in quantum Monte Carlo for a half-filled system with orbital degeneracy, although it seems that the orbital degenerate system is even slightly better described by RPA. Away from half-filling, RPA essentially misses to describe the steep rise of the response with $U$ and consequently fails to describe the screening even for surprisingly small values of $U$: Already for $U \gtrsim 3$ the absolute error exceeds 0.15 (relative error $\gtrsim 30\%$).
III. INTERPRETATION

A. Doping dependence

It is clear from Fig. 5 that the response strongly depends on the electron density $n_\sigma$. Obviously, for the completely empty ($n_\sigma = 0$) or the completely filled ($n_\sigma = 1$) system there is no response at all, while for half filling ($n_\sigma = 1/2$) screening breaks down at the Mott transition. In-between the response has a maximum. Since this maximum, as a function of electron density, is most pronounced for large $U$, we will consider the screening in that limit. For concreteness, we consider a system with $n_\sigma < 1/2$. Then, for large $U$, there will only be empty or singly occupied sites. In response to an external perturbation these electrons and holes will rearrange. Clearly, if there are no electrons ($n_\sigma$ close to zero) or no holes ($n_\sigma$ close to one) there is no room for rearrangement, so the response will be very weak. In the other extreme, for quarter filling, all electrons and holes can participate in the screening. More generally, for the screening of a plane wave with nonzero wave vector, the same number of electrons and holes have to participate in the response, so the response is limited by the density of electrons/holes, whichever is smaller. For $n_\sigma > 1/2$ the argument is analogous, simply replace empty by singly occupied sites and singly occupied by doubly occupied sites. We thus expect the response to be strongest around $n_\sigma = 1/4$ and $3/4$, which is roughly what is found in the calculations. There is of course also the prominent effect of the van Hove singularity, which greatly enhances the response and accounts for a shift in the position of the screening maximum, as well as for the strong asymmetry around half-filling.

B. Overscreening

In order to understand the overscreening we also consider the limit of large $U$. Again, for a system with less than half filling ($n_\sigma < 1/2$) there will only be singly occupied and empty sites. If the test charge is positive, the electrons will see a repulsive potential $cU$. Configurations with an electron on the site with the test charge will therefore be avoided (see Fig. 6): Moving the electron from that site to some other empty site results in a gain in potential energy $cU$, at no cost in interaction energy. Thus vacating the site with the test charge merely costs kinetic energy. Since for large $U$ the potential energy will eventually dominate, in the large-$U$ limit, the site with the repulsive test charge will be empty. This implies (i) that for a small perturbation $c$ the response will be larger than the perturbation (overscreening) and (ii) the response is (almost) independent of the perturbation ($\Delta n = \bar{n}$). But this means that the response is highly nonlinear: while in linear response one expects $\Delta n/c \approx dn/dc$ or, equivalently, $\Delta n \propto c$, in the limit $U \to \infty$ we expect that $\Delta n$ is constant, independent of $c$! We will further explore this nonlinearity in the next section.

There are two questions that come to mind. First, also RPA describes screening as the interplay between potential and kinetic energy. So why is there no overscreening in RPA? The answer is that in RPA the electron-electron interaction is described by a mean-field: An electron interacts with the mean electron density. So in going through the argument from above, we have to also account for the fact that removing an electron from the site with the test charge increases the mean electron density on the other sites, consequently increasing the mean-field interaction energy. Since, for the infinite system, this increase scales the same way as the gain in potential energy, RPA can give at most perfect screening: For a system with $M$ sites, neglecting the kinetic energy, we have

$$E/U = \frac{1}{2}(\bar{n} - \Delta n)^2 + \frac{M - 1}{2} \left( \bar{n} + \frac{\Delta n}{M - 1} \right)^2 + c(\bar{n} - \Delta n),$$

which is minimized for $\Delta n = (M - 1)/M \bar{n}$. The second question concerns the stability of the system. The perturbing charge induces the system to deviate from its homogeneous density in order to counteract the perturbation. But overscreening means that the resulting electron density becomes even more inhomogeneous than the perturbation, while naively one would expect that screening tends to restore as much as possible a homogeneous density. So does overscreening mean that the system prefers an inhomogeneous charge distribution, i.e. that it is unstable against formation of, e.g., a charge density wave? The answer is, of course, no. Forming an inhomogeneous charge density costs at least some kinetic energy. So only when this cost is compensated by a gain in potential energy, due to the interaction with the perturbing charge, will the charge density become inhomogeneous.

![FIG. 6. Screening of a point charge $c$ in the large-$U$ limit for less than half filling. Given a positive test charge $c$ the system will gain potential energy $cU$ by emptying the site with the test charge. Since there are empty sites in the system, no double occupancy needs to be created, so there is no cost in interaction energy. Thus vacating the site merely costs kinetic energy. Therefore, if $U$ is very large, an empty test-site is favorable: $\Delta n = \bar{n}$, independent of the perturbation $c$.](image)
of the order of unity or larger, it will even pay to create a double occupancy, since the gain in potential energy ($cU$) exceeds the cost in interaction energy ($U$); then $\Delta n = 2 - \bar{n}$. Systems with more than half filling can be discussed in just the same way. In that case there is complete screening for $c < 0$ by putting a double occupancy on the site with the test charge. For $1 > c > 0$ the test site will be singly occupied, while for $c > 1$ it will even pay to empty it at the expense of creating an additional double occupancy.

At half filling, in the large-$U$, limit all sites will be singly occupied and for $|c| < 1$ there will be no response at all ($\Delta n = 0$), since moving charge from or to the test site would involve the creation of a double occupancy, costing an energy $U$. Clearly, this Mott insulator behavior is missed by the RPA. But it is interesting that at half-filling the random phase approximation fails for the opposite reason than in the doped case. In RPA the screening always involves a cost in interaction energy of $U\Delta n^2/2$, which, for half filling, underestimates the true cost $U$, while for the doped system it is strongly overestimated. Thus at half filling RPA overestimates the response, while for the doped system it is severely underestimated.

Finally, two points about the arguments given above might be worth mentioning. First, the complete-screening limits are, of course, nothing but a simple consequence of the Pauli principle. Second, in our arguments we have at no point used the spin of the electrons. Thus, as long as there are holes (for $n_\sigma < 1/2$) or non doubly occupied sites (for $n_\sigma > 1/2$) in the system, there will be overscreening and nonlinear response, even if the system is not paramagnetic.

C. Nonlinear screening

As we have argued above, the response to a test charge will, in the limit $U \to \infty$, become practically independent of the perturbation: No matter how small the test charge $c > 0$, the system (with $n_\sigma < 1/2$) will respond in the strongest possible way (complete screening), by vacating the test site ($n_i = 0$). For $c < 0$ and $n_\sigma < 1/2$ the system will first respond by putting a single electron on the test site ($n_i = 1$), while for $c < 1$ it will even occupy the site doubly ($n_i = 2$). The latter, again, is the strongest possible response — complete screening. Thus for large $U$ the response becomes more or less independent of the perturbation, implying a strong nonlinearity. To check this prediction, we have calculated the response to test charges ranging from $c = -2 \ldots 1$ by exact diagonalization.

The results, for a Hubbard model ($t' = 0$) on a $4 \times 4$ lattice with $N_e = 1$ and 5 (closed shell systems), are shown in Fig. 7. To emphasize the nonlinearity, we plot $\Delta n/c$. If the response was linear, this ratio would be constant (and equal to the derivative $dn/dc$). The deviations from the horizontal thus show the degree of nonlinearity. The horizontal line through unity in the plot marks perfect screening ($\Delta n = -c$), above the response is stronger than the perturbation (overscreening). The dotted lines give the large-$U$ limits discussed above. The curves labeled $n_i = 0$ and $n_i = 2$ give the complete-screening limit.

Clearly, with increasing interaction $U$ the response gets stronger, eventually showing overscreening. But at the same time also the nonlinearity of the response (the slope of the curve when passing through $c = 0$) increases. This is not surprising, since the curves for finite $U$ are constrained by the response in the large-$U$ limit. Given the complete-screening limit it is easy to see that overscreening is impossible for $c > \bar{n}$ and $c < \bar{n} - 2$. But this implies that, the stronger the overscreening, the more nonlinear the response has to be.

FIG. 7. Response to a point charge $c$ for a $4 \times 4$ Hubbard model ($t' = 0$) with $N_e = 1$ and 5 electrons (closed shell) calculated by exact diagonalization. $\Delta n$ is the induced electron density on the test-site. The full lines give the results for $U = 4, 6, 8, 10, 12, 14, 16$, with the response getting stronger with $U$. For linear response $\Delta n/c$ is independent of $c$, so deviations of the curves from the horizontal indicate the nonlinearity of the response. The horizontal line through unity indicates perfect screening, overscreening above the line. The limiting curves $(\bar{n} - n_i)/c$ are given by the dotted lines.
IV. CONCLUSION

We have calculated the static density response for the one-band Hubbard model using Slave-Bosons at the paramagnetic saddle-point. For finite doping we find overscreening, i.e. the response exceeds the perturbation. This can be understood in the limit of large Hubbard interaction $U$, since strong screening leads to a gain in potential energy which increases with $U$, while it merely costs kinetic energy, which is practically independent of $U$. While overscreening thus necessarily occurs for large $U$, we found that it actually already starts at surprisingly small $U$, in particular if the screening is enhanced by the van Hove singularity.

The existence of overscreening might be surprising, if one assumes the random phase approximation to give a reasonable description of the charge response. In RPA there can be no overscreening, because the interaction is treated in the mean-field approximation, which implies that screening always costs interaction energy, which increases with $U$. Therefore the maximum response possible in RPA is perfect screening, where the response just compensates the perturbation. By construction RPA works well when the kinetic energy is much larger than the interaction energy. Thus it works well for small $U$, while it necessarily fails at the Mott transition, where it fails to describe the break-down of the screening. Surprisingly, when doping the system away from half filling, RPA rapidly get worse, this time severely underestimating the response. In that sense the doped system does not behave more metallic and RPA-like. Instead its charge response more or less resembles what one would expect for a Wigner crystal, i.e. in the opposite limit, where the interaction dominates over the kinetic energy. Also a Wigner crystal should show overscreening, when the crystal is pinned at the site of a point-charge perturbation, at the expense of loosing the kinetic energy associated with moving the Wigner crystal as a whole. Clearly, the response in that case should also show the same characteristic nonlinearity as we have found for the Hubbard model.

There have been arguments against overscreening, based on the intuition that a system with a response exceeding the external perturbation would resemble an active device, in the sense of electrical network theory, and should not be possible. More formal analyses reveal, however, that overscreening in the charge response is indeed possible, and does not imply an instability. As we have pointed out above, overscreening does not imply that the system prefers an inhomogeneous charge density. It is only in the presence of the perturbation that the cost in kinetic energy for forming the inhomogeneous electron density is compensated by the gain in potential energy from screening the perturbation.

An interesting consequence of the overscreening is that it changes the sign of the effective interaction between external charges, i.e. in the case of the Hubbard model, in the overscreening regime external charges will experience a negative effective $U$. Moreover, we note that the overscreening becomes the stronger the closer the van Hove singularity is moved to the lower band edge — in tempting analogy with the increase of the transition temperature in the cuprates. There are, however, two important observations to be made about this effective interaction. First, of course, it only applies to external charges and not to the interaction between the electrons in the system. Second, the concept of an effective interaction only makes sense, when that interaction is to a good approximation independent of the charges under consideration, i.e. if the response is linear.

We have, however, seen that the charge response of the Hubbard model can become strongly nonlinear. This can again be understood in terms of our large-$U$ argument. In fact, it follows, that the stronger the response, the more nonlinear it has to become. In the extreme case the induced density becomes independent of the perturbation. It is therefore even possible to give strict limits on the strength of the perturbation up to which overscreening is possible. This nonlinearity has to be kept in mind, when using linear response functions, and diagrammatic expansions for the Hubbard model.

1 E. Koch, O. Gunnarsson, and R.M. Martin, Phys. Rev. Lett. 83, 620 (1999)
2 G. Kotliar and A.E. Ruckenstein, Phys. Rev. Lett. 57, 1362 (1986)
3 T. Li, P. Wölfle, and P.J. Hirschfeld, Phys. Rev. 40, 6817 (1989)
4 J.W. Rasul and T. Li, J. Phys. C: Solid State Phys 21, 5119 (1988)
5 M. Lavagna, Phys. Rev. B 41, 142 (1990)
6 P. Wölfle and T. Li, Z. Phys. B 78, 45 (1990)
7 T. Li, Y.S. Sun, and P. Wölfle, Z. Phys. B 82, 369 (1991)
8 T. Li, Phys. Rev. B 46, 9301 (1992)
9 R. Frésard and W. Zimmermann, Phys. Rev. B 58, 15288 (1998)
10 Th. Jolicoeur and J.C. Guillou, Phys. Rev. B 44, 2403 (1991)
11 E. Arrigoni and G.C. Strinati, Phys. Rev. Lett. 71, 3178 (1993)
12 E. Arrigoni and G.C. Strinati, Phys. Rev. B 52, 2428 (1995); E. Arrigoni and G.C. Strinati, Phys. Rev. B 52, 13707 (1995).
13 G. Seibold, E. Siegmund, and V. Hizhnaykov, Phys. Rev. B 57, 6937 (1998)
14 W. Ziegler, H. Endres, and W. Hanke, Phys. Rev. B 58, 4362 (1998); W. Ziegler, PhD-Thesis, Universität Würzburg, 1996.
15 L. Lilly, A. Muramatsu, and W. Hanke, Phys. Rev. Lett. 65, 1379 (1990); L. Lilly, PhD-Thesis, Universität Würzburg, 1991.
16 R. Preuss, A. Muramatsu, W. von der Linden, P. Dieterich, F.F. Assaad, and W. Hanke, Phys. Rev. Lett. 73, 732 (1994)
17 W. Zimmermann, R. Frésard, and P. Wölfle, Phys. Rev. B 56, 10097 (1997)
18 H.-B. Schützler, C. Gröber, H.G. Evertz, and W. Hanke, cond-mat/9805133 and cond-mat/0104300
19 R. Hlubina, S. Sorella, and F. Guinea, Phys. Rev. Lett. 78, 1343 (1997)
20 D. Pines and P. Nozières: The Theory of Quantum Liquids, W.A. Benjamin, 1966.

21 D.A. Kirzhnits: The critical Temperature of a Superconducting System, in V.L. Ginzburg and D.A. Kirzhnits (Eds.), High-Temperature Superconductivity, Consultants Bureau, New York, 1982
22 D.A. Kirzhnits, Usp. Fiz. Nauk 119, 357 (1976) [Sov. Phys. Usp. 19, 530 (1976)]
23 O.V. Dolgov, D.A. Kirzhnits, and E.G. Maksimov, Rev. Mod. Phys. 53, 81 (1981)
24 E. Pavarini, I. Dasgupta, T. Saha-Dasgupta, O. Jepsen, and O.K. Andersen, cond-mat/0012051