T–Matrix Formulation of Impurity Scattering in Correlated Systems

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Using a generalized T–matrix description which, in principle, exactly includes Coulomb correlations and potential scattering events, resonant and bound impurity states are discussed. Like in the non-interacting case, the effects of the scattering potential can be divided into different partial wave channels, exploiting the symmetry of the underlying lattice. Due to Coulomb correlations bare local (i.e. s-wave) potentials become dynamic and extended, being responsible also for p-, d-wave etc. scattering effects. Numerically exact results for both the two-dimensional t–J and Hubbard models are used to construct a simple (static) approximation to the effective impurity potential which is shown to reproduce the exact resonant scattering and bound states in the relevant symmetry channels.

Experimental data on high–$T_c$ materials including substitutional defects serve for probing their unusual normal state properties as well as the nature of the superconductive phase. Introducing, for example, Zn in the copper oxide planes influences transport and magnetic properties and leads to a drastic reduction of the transition temperature $T_c$. The physical conclusions drawn from the results are still controversial. For example, this is the case for the local magnetic moment induced by a non–magnetic impurity such as Zn in hole doped superconducting samples, which could lead to a magnetic pair breaking mechanism.

However, one common feature seems to be the spatially extended nature of the magnetic effects on the CuO–based high–$T_c$ compounds. From residual resistivity measurements one deduces large scattering cross sections of several lattice constants in diameter favoring strong potential scattering likely connected to d–wave pair breaking. On the theoretical side there has been work based on s–wave impurity scattering in anisotropic superconductors revealing the strong influence of non–magnetic impurities. In addition, calculations were carried out for d–wave superconductors with combined scattering by impurities and Coulomb correlations.

In this paper we focus on the interplay between strong correlations and local potential scattering. This situation can be ascribed to Zn$^{2+}$ impurities with a filled (3d)$^10$ shell in the cuprate superconductors. We derive a microscopic picture of the mediated scattering processes using a generalized T–matrix description which exactly includes Coulomb correlations and which exploits the symmetries of the underlying lattice. Partial–wave phase shifts are introduced which, like in the non–interacting case determine the additional density of states caused by the impurity potential. For this purpose we take advantage of numerical exact results of translational–invariant lattices and combine them in analytical T–matrix expressions for a single impurity. By doing this we can determine the effective potential strengths acting in a perturbed t–J system investigated earlier.

Consider a correlated two-dimensional system such as the one band Hubbard model with Hamiltonian,

$$ H = H_0 + H_U = -t \sum_{\langle i,j \rangle} c_{i \sigma}^\dagger c_{j \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow}, $$

(1)

using standard notations, and a bare impurity operator

$$ V_{\text{Imp,} \sigma}(\delta \sigma) = \sum_{\delta \sigma} (t 0 \sigma 0 \sigma \epsilon_{\delta \sigma} + \text{h.c.}) \sum_{\sigma} V_{0 \sigma}^\text{bare} n_{0 \sigma}. $$

(2)

Here the four bonds connected to the impurity site at the origin are modified by $t_0$. The simplest description of a vacancy is then obtained by setting $t_0 = t$. For the sake of simplicity the potential is restricted here to the central site but the following analysis is more general and valid for extended one-body potentials. The above scattering problem on a lattice is defined spin–dependent and can therefore be adapted to different physical scenarios. In the case of non–interacting systems, e.g. $U = 0$, successive scattering is described by the Greens function $G_\sigma = G_0 + G_0 T_\sigma G_0$. Here, the T–matrix, defined as in usual scattering theory, $T_\sigma = V_{\text{Imp,} \sigma} \left(1 - G_0 V_{\text{Imp,} \sigma}\right)^{-1}$, involves only the unperturbed propagator $G_0$ and the bare potential $V_{\text{Imp,} \sigma}$.

On the other hand, for correlated systems it is {	extit{ad hoc}} not clear how to define a T–matrix leading to a similar result for the exact Greens function $G$. This can be achieved by investigating the representation of $G$ extracted from perturbation theory. For finite temperatures, the exact Greens function $G$ can be written in the Matsubara formalism and in momentum space as

$$ G_\sigma^{-1}(k, k', \omega_n) = i \omega_n - \epsilon(k) - \Sigma_\sigma(k, k', \omega_n). $$

(3)

The self–energy $\Sigma$ is a sum of three terms $\Sigma_U(k, k', \omega_n), \Sigma_{U/V,\sigma}(k, k', \omega_n)$ and $V_{\text{Imp,} \sigma}(k, k')$. In a diagrammatic
Greens function of the system is given by the trace over the retarded
\( \alpha \) active phase of these
impurity and an additional impurity–caused contribution
determinant of the T–matrix factorizes into the subdeter-
lifetime of these states.

determine the additional density of states (DOS) caused
at the bound state energies \( \omega \).

symmetry of the lattice
to the symmetrized states of the underlying point-group
formation of its matrix elements in real space according
also for
interactions. Here we adopt a somewhat simpler approach by
showing that a crude static but nevertheless interaction–
dependent Ansatz can be made for \( V_{eff,\sigma} \) which can
describe, within reasonable accuracy, the scattering pro-
cesses. This method enables us to understand in more
physical terms the interplay between the interaction and
short-range impurity scattering.

One important feature which has to be included in the
Ansatz is the longer range character of \( V_{eff} \) due to the
background of the correlated host. This can simply be
seen from the connection between the bare and the
dynamically modified potential. By explicitly transforming the
Coulomb term to the real-space irreducible repre-
sentation, one finds local interactions between different
wave–symmetries, i.e.

\[
H_U = \sum_{\nu,\alpha,\beta,\gamma,\delta} U_{\alpha,\beta,\gamma,\delta}^{\nu,\omega,\alpha,\gamma} c_{\alpha,\gamma}^\dagger c_{\beta,\delta}^\dagger c_{\gamma,\delta} c_{\beta,\gamma} \quad \text{ (8)}
\]

where \( c_{\alpha,\nu}^{(t)} \) are the symmetrized annihilation (creation)
operators of the one–particle spin (\( \sigma \)) states. \( \alpha \) labels
in general all irreducible representations of the site–type

Note that, although it contains \( \alpha \)-wave operators
the above expression for \( H_U \) is invariant under all the
point group symmetries. This implies selection rules on
the matrix elements \( U_{\alpha,\beta,\gamma,\delta}^{\nu,\omega,\alpha,\gamma} \) which, for simplicity, are
not specified here. Therefore, even for a pure \( s \)-wave
potential \( V_{bare}^{\nu,\omega,\alpha,\gamma} \alpha,\gamma \) at the origin, incoming \( d \)-wave
propagators are scattered at \( \nu = 1 \) from a potential med-
ated by the Coulomb repulsion as shown in Fig. 1.

This demonstrates that, due to many–body effects,
even local (\( s \)-wave) potentials always become dynami-
cally extended, being in general responsible for scattering
contributions in all symmetry channels. In our numer-
ical results the effective potential in Eq.(4) is described
by assuming the following static approximation for the
effective potential in Eq.(4);

\[
V_{eff}^{stat} = t' \sum_{\sigma} (e_{\sigma,\gamma}^{\dagger} c_{\sigma,\gamma}^\dagger + h.c.) + \sum_{\nu,\sigma} V_{\nu,\sigma}^{\alpha,\gamma} c_{\nu,\sigma}^\dagger c_{\nu,\sigma}^\dagger \quad \text{ (9)}
\]

Generally, the \( \nu \)-off–diagonal (diagonal) part of \( V_{eff} \)
also takes into account the effective change of the hopping
amplitudes (potential terms).

Next, we proceed with our numerical results. At zero
temperature, the retarded Greens function $G_\nu$ appearing in the above equations is calculated by exact diagonalization (ED) techniques for the half-filled 2D $t$–$J$ model. In this context, we regard this model as the strong–coupling limit of our original Hamiltonian Eq.(1) to perform the T–matrix calculations (i.e. $J = 4t^2/U$).

We consider the situation of reference where an inert site to the lattice restores the spin–degeneracy of the system, leading also to an antiferromagnetic structure in the vicinity of the impurity which would lead again to spin–independent effective potentials. Keeping in mind, that we restrict our calculations to the low–lying excitations in the above mentioned singlet channel, we omit spin indices from now on. For the case of interest here ($t_0 = t$ or more generally for $t_0 = 0$) the problem becomes particle-hole symmetric. Then, for simplicity, we define $\omega = 0$ as the lower edge of the quasiparticle band of the $t$–$J$–model (lower Hubbard band). In the hole representation, positive (negative) values of $V^0_{\nu 0,1,2}$ correspond to repulsive (attractive) potentials.

According to the local DOS results of Ref.23, the values of $V^0_\nu$ are set to large values $\sim 20t$ in order to express particles from the corresponding site–types $\nu = 0, 2$. In our calculations $t'$ increases the bound-state energy quadratically. Taking the actual small binding energies of $t'$ into account the small parameter $t'$ is therefore set to zero. In this sense the derived potential strengths represent an upper limit.

Fig. 2 displays the exact bound state energies $\omega_{B\nu}$, calculated from the local DOS $D_\nu$ for a 20–site cluster with an isolated site at the origin. By using the T–matrix, the energetic locations of the bound states are reproduced for values of $J = 0.5$ and $J = 1.0$ fixing the effective potentials $V^0_\nu$. Fig. 2 also exhibits the dependence of $V^0_\nu$ on the exchange coupling $J$ of the unperturbed system. As one expects, the attractive potentials increase with $J$. One finds the actual value of the effective potential to be of the order of $J$, which is the loss of magnetic energy per bond of the inert site.

Due to the dynamic renormalization, the potential $V^0_\nu$ acts, as mentioned, differently in each symmetry sector being largest for the $s$–wave channel. Note that in the limit of vanishing interaction strength ($U \to 0$), the $p$– and $d$–wave potentials also have to vanish, reflecting non–extended potential scattering. Therefore, in an interacting system, there should exist an optimum correlation strength producing the largest effective potentials for bound states.

For $J = 0.5$ Fig. 3a) shows the DOS of the unperturbed 26–site cluster used to calculate the additional impurity–induced density in Fig. 3b). Assuming the effective potentials to be slowly varying functions of $\omega$ one finds a suppression of density for small energies in agreement with the exact result in Fig. 3c).

Now, we investigate scattering in the 2D Hubbard model. For finite temperatures, we exploit results of Quantum Monte Carlo (QMC)/Maximum Entropy calculations for the undoped system by inserting the unperturbed Greens functions into the T–matrix equations.

At half–filling and for $U = 8t$, $\beta t = 10$, we use the effective potentials derived from the $t$–$J$–model for $J = 4t^2/U = 0.5$ and for the particle-hole symmetric case $t_0 = t$. In this case, $V^0_{\nu \bar{\nu}}$ is irrelevant and can be set to zero, while the effective potentials change sign at the chemical potential $\mu$. Both pure systems are characterized by long–range antiferromagnetic correlations being disrupted by the impurity which should lead to a similar behavior regarding the formation of bound states. Actually, the states appearing below the $t$–$J$ quasiparticle band are now located just above the small dispersive quasiparticle band of width $\sim 2J$ sitting on top of a several $t$ wide incoherent background. This can be seen in Fig. 4 displaying the unperturbed DOS $D_U$ obtained from QMC calculations and the (non–normalized) additional density $\Delta D_{\alpha}$. Differing from the $t$–$J$–case the s-wave contributions are shifted towards the quasiparticle band. The appearance of these states results in an overall effect of narrowing the gap of the unperturbed Hubbard model by almost 20%.

In summary, we have considered a formally exact T–matrix method adapted to correlated systems which revealed the many–body interactions as the origin of dynamically extended potentials. Using numerical data for the unperturbed propagators, we reproduced the static effective potentials causing bound states in a 2D $t$–$J$–lattice with an inert site. Applying the formalism to the insulating 2D Hubbard model, we have shown the correspondence of the two models regarding the appearance of spectral weight in the correlation gap. Our result is relevant for T–matrix approximations in the dilute impurity limit, i.e. where the single impurity scattering has to be treated exactly. There, higher symmetry channels than the usually considered s–wave contributions have to be taken into account for interacting systems. Our static, effective potentials in Eq.(9) can, for example, directly be used as an input to a cluster diagonalization approach, where the effect of potential impurity scattering in a 2D superconductor described by a BCS mean–field theory is studied. In ref.23 the impurity potential was parameterized. Nevertheless, already this work demonstrated that the range of the impurity potential is of quantitative importance in the case of strong potential scatterers.

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20 For the $C_{4V}$–lattice of the Hubbard model there exist in general five different representations. At the considered impurity site–types $\nu = 0, 1, 2$, only $s$–, $p$– and $d$–wave representations contribute. The $p$–wave is degenerated ($p_x = p_y$). Different site–types $\nu$ are distinguished by their distance from the origin.
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FIG. 1: Typical lowest order diagrams for the self-energy: a) Local interaction vertex connecting different symmetry channels. b), c) Diagrams of $\Sigma_{UV}$ describing $d$-wave extended potential scattering of type 1; first order static contribution (b) and second order dynamic scattering process (c) in U. Scattering by the bare potential is depicted by a cross.
FIG. 2: Bound state energies $\omega_{BS}$ of an inert site in the $t$–$J$–model as a function of $J$ [17]. The effective potentials $V_{1}^{\alpha}$ causing these states, derived by the generalized T–matrix method from a 26–site cluster.
FIG3: a) Total density of states of the 26-site cluster without the impurity calculated exactly by ED. b) Additional density due to effective potentials at site types $\nu = 0, 1, 2$. d-wave: short–dashed lines, s-wave: solid lines, p-wave: long–dashed lines. c) Exact local density of states at site type $\nu = 1$ for a 20-site cluster with an inert site [17].
FIG. 4: Influence of effective potentials on the half-filled Hubbard model. $D_U$ from QMC calculations ($\beta t = 10$). The appearance of various symmetry bound states causes gap–narrowing at the edges of the Hubbard bands.