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Physikalisches Institut
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http://www.kroha.uni-bonn.de/teaching

Special Topics in Condensed Matter Theory
Winter term 2016/17

Exercise 4

(Solutions due on 9 December, 2016)

1. Bound states at an impurity potential (20 points)

In the lecture it was shown: Let $\Psi_\alpha^\dagger(t)$ be the creation operator for an electron in a single-particle state $|\alpha\rangle$, and let $G_\alpha(t) = -i\langle \hat{T}\Psi_\alpha(t)\Psi_\alpha^\dagger(0)\rangle$ be the corresponding Green's function for a particle in this state. If, as function of the frequency z, $G_\alpha(z)$ has a pole on the real frequency axis, then the lifetime of $|\alpha\rangle$ is infinite, i.e., $|\alpha\rangle$ is an eigenstate of the Hamiltonian.
We had shown this specifically for momentum eigenstates $|\vec{p}\rangle$. However, it is generally true, since the proof did not make use of a specific momentum state.

We now consider the Hamiltonian of an electron in a $d-$dimendional, periodic lattice with an impurity potential at site $\vec{r}=0$, $\tilde{V}(\vec{r}) = V\delta^d(\vec{r})$,

$$\hat{H} = \hat{H}^{(0)} + \hat{V} = \sum_{\vec{k}} \varepsilon_{\vec{k}} c_{\vec{k}}^\dagger c_{\vec{k}} + V c_0^\dagger c_0 \ ,$$

with the local creation operator at site $\vec{r}=0$, $c_0^\dagger = \sum_{\vec{k}} c_{\vec{k}}^\dagger$. Spin is not considered, for simplicity. We want to analyze the existence of bound states in this system.

From the above remark, a pole on the real axis in the *local* Green's function at a site $\vec{r}=0$,

$$G_0(t) = -i\langle \hat{T} c_0(t) c_0^\dagger(0)\rangle$$

indicates a bound state at that site.

a) Consider the impurity $\hat{V}$ as a perturbation and expand the Dyson series for the (full), local Green's function $G_0(\omega)$ in terms of the bare, local Green's function $G_0^{(0)}(\omega)$. Sum up this infinite series in the form of a Dyson equation for $G_0(\omega)$.
[Result: $G_0 = G^{(0)}/(1 - VG_0^{(0)})$]

b) We now consider a 2-dimensional system. In $d=2$ dimensions, the density of states (DOS) has a step at the band edges (see exercise sheet 3). It can, therefore, be modelled for a lattice with upper and lower band edges by

$$N(\omega) = \frac{1}{2D}\Theta(D - |\omega|) \ ,$$

where D is the half bandwidth.

Use the relation of the imaginary part of the retarded Green's function to the DOS to calculate $\mathrm{Im}G^{(0)R}(\omega)$ and then $\mathrm{Re}G^{(0)R}(\omega)$ via the Kramers-Kronig relation.

Use the result of a) to analyze under which condition the impurity potential has a bound state. Determine the binding energy of the bound state below/above the band edges (position of the pole), if it exists.

c) We now consider a 3-dimensional system. In a $d = 3$ dimensional lattice, the DOS can generally be modelled by

$$N(\omega) = \frac{2}{\pi D}\sqrt{1 - (\omega/D)^2}\ ,$$

(see exercise sheet 3; note the normalization).

Repeat the analysis of b) for the $d = 3$ dimensional system. Is there always a bound state for an attractive potential ($V < 0$) in $d = 3$ dimensions?

d) Alternatively, the Dyson equation of a) can be derived by means of equations of motion. Derive the equations of motion for $G_0^{(0)}(t)$ and $G_0(t)$ and use them to write down the Dyson equation for $G_0(\omega)$ (as function of energy ω).