Theorie der Kondensierten Materie II SS 2017

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Blatt 1
Lösungsvorschlag

1. Scattering Amplitude:

The scattering state

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}} + \chi_{\vec{k}}(\vec{r}), \quad \chi_{\vec{k}}(\vec{r}) = f(\vec{k}, k\vec{n})\frac{e^{ik|\vec{r}|}}{|\vec{r}|},$$

can be found from the Green's function formalism as follows.

First, one can write down the Schrödinger equation describing a particle moving in a given potential $V(\vec{r})$ in the momentum representation with the help of the single-particle Green's function:

$$\left[\hat{G}_0^{-1} - \hat{V}\right]\psi_{\vec{k}}(\vec{r}) = 0.$$

Recall, that in the momentum representation the free-particle Green's function is

$$\hat{G}_0 = \frac{1}{\epsilon - \vec{p}^{\,2}/(2m) + i\delta},$$

while the potential $\hat{V}$ is actually an (integral) operator.

Substituting the above scattering wave function and noticing that the plane wave is a solution of the Schrödinger equation for a free particle, one finds

$$\left[\hat{G}_0^{-1} - \hat{V}\right]\chi_{\vec{k}}(\vec{r}) = \hat{V}e^{i\vec{k}\vec{r}} = \hat{V}|\vec{k}\rangle.$$

The solution can be formally written don using the "full" Green's function

$$\hat{G}^{-1} = \hat{G}_0^{-1} - \hat{V} \quad \Rightarrow \quad \chi_{\vec{k}}(\vec{r}) = \langle\vec{r}|\hat{G}\hat{V}|\vec{k}\rangle.$$

Now, we can expand the Green's function into a power series

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{V}\hat{G}_0 + \ldots$$

This allows us to write the solution for $\chi_{\vec{k}}(\vec{r})$ as

$$\chi_{\vec{k}}(\vec{r}) = \langle\vec{r}|\hat{G}_0\hat{V} + \hat{G}_0\hat{V}\hat{G}_0\hat{V} + \ldots|\vec{k}\rangle = \langle\vec{r}|\hat{G}_0\hat{F}|\vec{k}\rangle,$$

where

$$\hat{F} = \hat{V} + \hat{V}\hat{G}_0\hat{V} + \ldots$$

This series can be pictorially represented by the diagrams shown in the original figure.

To relate the quantity $\hat{F}$ to the scattering amplitude, consider the following expression for the free-particle Green's function ($\epsilon = k^2/(2m)$)

$$G_0(\epsilon; \vec{r}, \vec{r}\,') = \int \frac{d^3p}{(2\pi)^3} \frac{e^{i\vec{p}(\vec{r}-\vec{r}\,')}}{\epsilon - \vec{p}^{\,2}/(2m) + i\delta} = -\frac{m}{2\pi} \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}.$$

Here the imaginary part $i\delta$ has the sign corresponding to the retarded function. The use of the advanced function would result in the series for the complex conjugated scattering amplitude.

Now we are going to consider this Green's functions "at large distances". The meaning of this phrase is the following. We choose the coordinate system in such a way that the scattering center is located near the origin, while the vector $\vec{r}$ points towards the observation point. The vector $\vec{r}\,'$ spans the area around the origin, where the potential $V(\vec{r}\,')$ is nonzero (in a scattering problem we are looking at a potential that is confined to a certain area and study how particles – or waves – arriving from infinity scatter off this potential). Now we denote the length of the vector $\vec{r}$ by R and assume all other lengths in the problem to be much smaller:

$$\vec{r} = R\vec{n}, \quad |\vec{r}-\vec{r}\,'| \approx R - |\vec{r}\,'| \cos\theta + \mathcal{O}(1/R), \quad \cos\theta = \frac{\vec{n}\cdot\vec{r}\,'}{r'},$$

where θ is the angle between $\vec{n}$ and $\vec{r}\,'$.

Substituting the above approximation into the single-particle Green's function, we find

$$\chi_{\vec{k}}(\vec{r}) = -\frac{me^{ikR}}{2\pi R} \int d^3r' e^{-ik|\vec{r}\,'|\cos\theta} \langle \vec{r}\,'|\hat{F}|\vec{k}\rangle.$$

Comparing this expression with the definition of the scattering amplitude, we find the relation

$$f(\vec{k}_1, \vec{k}_2) = -\frac{m}{2\pi} \langle \vec{k}_2|\hat{F}|\vec{k}_1\rangle,$$

where

$$\vec{k}_2 = \left|\vec{k}_1\right| \vec{n}.$$

Let us now derive the integral equation for the scattering amplitude. We re-write the series expantion for $\hat{F}$ in the momentum representation:

$$\hat{F} = \hat{V} + \hat{V}\hat{G}_0\hat{V} + \ldots \quad \Rightarrow \quad F(\vec{k}_1, \vec{k}_2) = F^{(1)}(\vec{k}_1, \vec{k}_2) + F^{(2)}(\vec{k}_1, \vec{k}_2) + \ldots$$

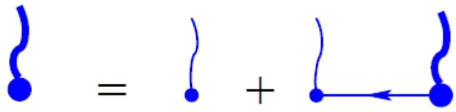
$$F^{(1)}(\vec{k}_1, \vec{k}_2) = V(\vec{k}_2 - \vec{k}_1),$$

$$F^{(2)}(\vec{k}_1, \vec{k}_2) = \int d^3q \frac{V(\vec{k}_2 - \vec{q})V(\vec{q} - \vec{k}_1)}{\epsilon - q^2/(2m) + i\delta}.$$

Now we can see, that in the series of diagrams in the figure the straight lines correspond to free-particle Green's functions and the curvy lines – to the matrix elements of the scattering potential. All internal momenta should be integrated over, while the incoming and outgoing momenta should be "on shell", i.e. should satisfy $\epsilon = k^2/(2m)$.

The integral equation for $\hat{F}$ can be easily expressed either diagrammatically, or in the operator form:

$$\hat{F} = \hat{V} + \hat{V}\hat{G}_0\hat{V} + \hat{V}\hat{G}_0\hat{V}\hat{G}_0\hat{V} + \cdots = \hat{V} + \hat{V}\hat{G}_0(\hat{V} + \hat{V}\hat{G}_0\hat{V} + \ldots) = \hat{V} + \hat{V}\hat{G}_0\hat{F}.$$



In the momentum representation the integral equation has the form

$$F(\vec{k}_1,\vec{k}_2) = V(\vec{k}_2-\vec{k}_1) + 2m\int \frac{d^3q}{(2\pi)^3}\frac{V(\vec{k}_2-\vec{q})F(\vec{k}_1,\vec{q})}{\epsilon - q^2/(2m)+i\delta}.$$

Solving this equation by iterations, we again find the series for the scattering amplitude.

2. Shallow well:

(a) In the previous exercise we have derived the following series for the scattering amplitude

$$\hat{F}(\vec{k}_1,\vec{k}_2) = \hat{V} + \hat{V}\hat{G}_0\hat{V} + \hat{V}\hat{G}_0\hat{V}\hat{G}_0\hat{V} + \dots$$

Here, both V and G_0 should be understood as "matrices" in the momentum space. The potential in momentum space is given by

$$V(\vec{k}_1,\vec{k}_2) = \int d^dr_1 d^dr_2 V(\vec{r}_1-\vec{r}_2)e^{-i\vec{k}_1\vec{r}_1+i\vec{k}_2\vec{r}_2}.$$

For the δ-potential $V(\vec{r}_1-\vec{r}_2)=V(\vec{r}_1)\delta(\vec{r}_1-\vec{r}_2)$ we find

$$V(\vec{k}_1,\vec{k}_2) = V(\vec{k}_1-\vec{k}_2).$$

The retarded Green's function G_0 in the momentum space is

$$G_0(\epsilon,\vec{k}_1,\vec{k}_2) = (2\pi)^d\delta(\vec{k}_1-\vec{k}_2)G_0(\epsilon,\vec{k}_1) = \frac{(2\pi)^d\delta(\vec{k}_1-\vec{k}_2)}{\epsilon-\epsilon_{k_1}+i\delta},$$

where $\epsilon_k = k^2/(2m)$.
As a result, the scattering amplitude can be also treated as a function of ϵ:

$$F(\epsilon,\vec{k}_1,\vec{k}_2) = V(\vec{k}_1-\vec{k}_2) + \int\frac{d^dq}{(2\pi)^d}V(\vec{k}_1-\vec{q})G_o(\epsilon,\vec{q})V(\vec{q}-\vec{k}_2)+\dots$$

In contrast to the previous exercise, here we are not taking the "on-shell" solution $F(\epsilon)=F(\epsilon_k)$, but consider ϵ as an independent variable.
The expansion for the full Green's function can now be expressed in terms of the scattering amplitude

$$G = G_0 + G_0VG_0 + G_0VG_0VG_0 + \dots = G_0 + G_0FG_0.$$

The eigenstates of the system can be found from the poles of the Green's function. Hence, if the scattering amplitude had a pole at some negative vale of ϵ, this would indicate a bound state.

(b) Let us re-write the series for the scattering amplitude in the form of an integral equation:

$$\hat{F} = \hat{V} + \hat{V}\hat{G}_0\hat{V} + \hat{V}\hat{G}_0\hat{V}\hat{G}_0\hat{V} + \cdots = V + VG_0F,$$

which explicitly corresponds to

$$F(\epsilon, \vec{k}_1, \vec{k}_2) = V(\vec{k}_1 - \vec{k}_2) + \int \frac{d^d q}{(2\pi)^d} V(\vec{k}_1 - \vec{q}) G_0(\epsilon, \vec{q}) F(\epsilon, \vec{q}, \vec{k}_2).$$

Approximating the well by a δ-function potential

$$V(\vec{r}) = -a^d U_0 \delta(\vec{r}), \qquad V(\vec{q}) = -\int d^d r e^{-i\vec{q}\vec{r}} V(\vec{r}) = -a^d U_0.$$

As a result, the integral equation fro the scattering amplitude is

$$F(\epsilon, \vec{k}_1, \vec{k}_2) = -a^d U_0 - a^d U_0 \int \frac{d^d q}{(2\pi)^d} G_0(\epsilon, \vec{q}) F(\epsilon, \vec{q}, \vec{k}_2).$$

Solution of this equation are only possible if the scattering amplitude is independent of both momenta. Then

$$F(\epsilon) = -a^d U_0 \left[1 + F(\epsilon) \int \frac{d^d q}{(2\pi)^d} G_0(\epsilon, \vec{q})\right],$$

and hence

$$F(\epsilon) = -\frac{a^d U_0}{1 + a^d U_0 \int \frac{d^d q}{(2\pi)^d} G_0(\epsilon, \vec{q})}.$$

The remaining calculations we will perform separately in each dimensionality.

d=1

$$\int \frac{dq}{2\pi} G_0(\epsilon, \vec{q}) = \int \frac{dq}{2\pi} \frac{1}{\epsilon - q^2/(2m) + i0}.$$

Since we are looking for a bound state at some negative energy, then there is no pole in this integral and we can drop the imaginary $i0$. Denoting $\chi^2 = -2m\epsilon$, we find

$$\int \frac{dq}{2\pi} G_0(\epsilon, \vec{q}) = -2m \int \frac{dq}{2\pi} \frac{1}{q^2 + \chi^2} = -\frac{m}{\chi}.$$

In this case, the scattering amplitude is given by

$$F(\epsilon) = -\frac{aU_0}{1 - aU_0 m/\chi}.$$

The pole corresponds to the bound state energy

$$\epsilon = -ma^2 U_0^2/2.$$

d=2 Repeating the same argument in two dimensions we arrive at the logarithmically divergent integral

$$\int \frac{d^2q}{(2\pi)^2} G_0(\epsilon, \vec{q}) = -2m \int\limits_0^\infty \frac{qdq}{2\pi} \frac{1}{q^2 + \chi^2}.$$

To regularize the divergence, we recall that the approximation $V(\vec{q})$ is valid only for $q < 1/a$. For larger q the potential falls off rapidly. Neglecting this contribution we find

$$\int \frac{d^2q}{(2\pi)^2} G_0(\epsilon, \vec{q}) = -2m \int\limits_0^{1/a} \frac{qdq}{2\pi} \frac{1}{q^2 + \chi^2} \approx \frac{m}{\pi} \ln(a\chi).$$

As a result, the scatteing amplitude has the form

$$F(\epsilon) = -\frac{aU_0}{1 + a^2 U_0 m \ln(a\chi)/\pi}.$$

The pole corresponds to the exponentially small bound state energy

$$\epsilon = -\frac{1}{2ma^2} e^{-2\pi/(ma^2 U_0)}.$$

This result was obtained with the so-called "logarithmic accuracy": since we have only estimated the momentum integral, the exponent is valid up to a factor of order unity.

d=3 Now the momentum integral has the form

$$\int \frac{d^3q}{(2\pi)^3} G_0(\epsilon, \vec{q}) = -2m \int\limits_0^\infty \frac{q^2dq}{2\pi^2} \frac{1}{q^2 + \chi^2}.$$

This integral still diverges at large q, but in contrast to the lower dimensions it converges at small q even in the limit $\chi \to 0$. Then we can estimate the upper bound by setting χ to zero:

$$I_3(\epsilon) = \left| \int \frac{d^3q}{(2\pi)^3} G_0(\epsilon, \vec{q}) \right| \approx 2m \int\limits_0^{1/a} \frac{q^2dq}{2\pi^2} \frac{1}{q^2 + \chi^2} \leqslant \frac{m}{\pi^2 a}.$$

This yields the following result for the scattering amplitude

$$F(\epsilon) = -\frac{aU_0}{1 - a^3 U_0 I_3(\epsilon)}.$$

The last term is small

$$a^3 U_0 I_3(\epsilon) \leqslant m a^2 U_0/\pi^2 \ll 1$$

and hence there is no pole.

(c) The obtained results coinside with those obtained by standard quantum-mechanical methods.

3. Friedel oscillations:

(a) We begin with the Green's function in the momentum representation

$$G_{\alpha\beta}(\epsilon, q) = \frac{\delta_{\alpha\beta}}{\epsilon - q^2/(2m) + \mu + i0\text{sign}\epsilon}.$$

The Fourier transform to the coordinate space can be performed as follows

$$G_{\alpha\beta}(\epsilon, x - x') = \delta_{\alpha\beta} \int \frac{dq}{2\pi} \frac{e^{iq(x-x')}}{\epsilon - q^2/(2m) + \mu + i0\text{sign}\epsilon}.$$

Since $G(\epsilon, x, x') = G(\epsilon, x', x)$ it is sufficient to consider $x > x'$. Then we should close the integration contour in the upper half-plane of complex q.
The integrand has two poles at

$$q_\pm = \pm\sqrt{2m(\epsilon + \mu) + i0\text{sign}\epsilon}.$$

For positive $\epsilon > 0$, the pole q_+ is in the upper half-plane (i.e. has the positive infinitesimal imaginary part), such that

$$G_{\alpha\beta}(\epsilon, x - x') = -i\delta_{\alpha\beta} \frac{m}{q_+} e^{iq_+|x-x'|}.$$

(b) In the presence of the boundary the space in ho longer homogeneous. Therefore, the Green's function is no longer a function of only the difference of the coordinates.
The easiest way to define the Green's function is to use the method of images known from the electrostatics:

$$G(\epsilon, x, x') = G_0(x - x') - G_0(x + x'),$$

where G_0 is the Green's function in the infinite space considered in the previous exercise.
The formal proof of this method consists in using the fom of the Lehman expansion for the Gree's function

$$G(\epsilon, x, x') = \sum_\alpha \frac{\psi_\alpha(x)\psi_\alpha^\dagger(x')}{\epsilon - q^2/(2m) + \mu + i0\text{sign}\epsilon},$$

where $\psi_\alpha(x)$ are the single-particle wavefunctions. In the infinite space, these functions are the plain waves, hence the usual Fourier relation between the momentum and coordinate representations. On the half-line, the wave functions are sines (see the next exercise). Expressing the sines in terms of the exponentials, one can easily derive the same result as above, justifying the method of images.

(c) The wavefunctions of free electrons in the presence of the boundary are no longer plain waves. The functions satisfying the boundary condition are

$$\psi_k(x) = \sqrt{\frac{2}{L}} \sin kx.$$

The particle density is then given by

$$n(x) = 2\frac{2}{L} \sum_{k<k_F} \sin^2 kx = \frac{4}{\pi} \int_0^{k_F} dk \sin^2 kx = \frac{2}{\pi} \left[k_F - \frac{\sin k_F x}{2x} \right].$$

Same result can be obtained from the Green's function found in the previous exercise (3b).