Karlsruher Institut für Technologie | Institut für Theorie der Kondensierten Materie

Theorie der Kondensierten Materie II SS 2015

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Blatt 2
Lösung

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1. Shallow well:

A "shallow well" is a potential well with the depth $U_0 \ll \hbar^2/(2ma^2)$, where a is the width (or radius) of the well. In such a potential, the energy of a bound state is much smaller than the well depth U_0, while its wave function extends over distances much greater than the well radius a.

Consider a shallow well in a D-dimensional space and find out in which case do the bound states exist.

(a) **Show, that the energy of each bound state corresponds to a pole of the scattering amplitude $F(\vec{k}_1, \vec{k}_2)$ as a function of energy.**

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

$$F(\vec{k}_1, \vec{k}_2) = V + VG_0V + VG_0VG_0V + \ldots$$

Both V and G_0 should be understood as matrices in $\vec{k}$ space. Since in the $\vec{r}$ space $V(\vec{r}_1, \vec{r}_2) = V(\vec{r}_1)\delta(\vec{r}_1 - r_2)$ we obtain for the $\vec{k}$ space

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

For the (retarded) Green's function we have

$$G_0(\epsilon, \vec{k}_1, \vec{k}_2) = (2\pi)^D \delta(\vec{k}_1 - \vec{k}_2) G_0(\epsilon, \vec{k}_1) = (2\pi)^D \delta(\vec{k}_1 - \vec{k}_2) \frac{1}{\epsilon - \epsilon_{k_1} + i\delta} \ .$$

Here $\epsilon_k \equiv \hbar^2 k^2/2m$. Thus, formally, F is also a function of frequency

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

In the previous exercise we considered the scattering states and we had to take the on-shell solution

$$F(\vec{k}, k\vec{n}) = F(\epsilon = \epsilon_k, \vec{k}, k\vec{n}) \ .$$

Now we consider ϵ as independent.

The expansion for the full Green's function can be written as follows

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

Poles of $G(\epsilon, \vec{k}_1, \vec{k}_2)$ as a function of ϵ correspond to the eigenstates of the problem. Thus, if F would have a pole at negative ϵ this would mean an bound state.

(b) **Show, that bound states in shallow wells exist only for $D \leqslant 2$.**
The series for F can be rewritten as follows

$$F = V + VG_0V + VG_0VG_0V + \cdots = V + VG_0F \ .$$

This gives

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

For $V(\vec{r})$ approximated as $V(\vec{r}) = -a^D U_0 \delta(\vec{r})$ we obtain

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

Thus

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

This equation can only be consistent if F is independent of both $\vec{k}_1$ and $\vec{k}_2$. This gives

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

and

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

1) For $D = 1$ we obtain

$$\int \frac{d^Dq}{(2\pi)^D} G_0(\epsilon, \vec{q}) = \int \frac{dq}{2\pi} \frac{1}{\epsilon - \frac{\hbar^2 q^2}{2m} + i0} = -\frac{2m}{\hbar^2} \int \frac{dq}{2\pi} \frac{1}{q^2 + \chi^2} \ ,$$

where $\chi^2 \equiv -2m(\epsilon + i0)/\hbar^2$. Since we are interested in $\epsilon < 0$, we have $\chi^2 > 0$ and we can safely drop $i0$. Thus,

$$\int \frac{dq}{2\pi} \frac{1}{\epsilon - \frac{\hbar^2 q^2}{2m} + i0} = -\frac{2m}{\hbar^2} \int \frac{dq}{2\pi} \frac{1}{q^2 + \chi^2} = -\frac{m}{\hbar^2 \chi} \ ,$$

$$F(\epsilon) = \frac{-aU_0}{1 - \frac{aU_0 m}{\hbar^2 \chi}} = \frac{-aU_0}{1 - \frac{aU_0 m}{\hbar\sqrt{-2m\epsilon}}} \ .$$

The pole is at

$$\epsilon = -\frac{ma^2 U_0^2}{2\hbar^2} \ . \tag{1}$$

2) For $D = 2$ we obtain

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

The integral is logarithmically divergent. We must regularise it by noting that the approximation $V(\vec{q}) = -a^D U_0$ is only valid for $q < 1/a$. For $q > 1/a$ the potential $V(\vec{q})$ vanishes rapidly. Thus

$$\int \frac{d^Dq}{(2\pi)^D} G_0(\epsilon, \vec{q}) = -\frac{2m}{\hbar^2} \int_0^{1/a} \frac{qdq}{2\pi} \frac{1}{q^2 + \chi^2} \approx \frac{m}{\pi\hbar^2} \ln(a\chi) \ . \tag{2}$$

Finally,

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

The pole is at

$$\epsilon = -\frac{\hbar^2}{2ma^2} e^{-\frac{2a^2 U_0 m}{\pi \hbar^2}} \ .$$

Of course the coefficient in the exponent could be multiplied by $O(1)$ since the integral in (2) is only an estimate.

3) For $D = 3$ we obtain

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

This integral behaves regularly at $\chi \to 0$ and we can estimate

$$I_3(\epsilon) \equiv \left| \int \frac{d^D q}{(2\pi)^D} G_0(\epsilon, \vec{q}) \right| = \frac{2m}{\hbar^2} \int_0^{1/a} \frac{q^2 dq}{2\pi^2} \frac{1}{q^2 + \chi^2} \leq \frac{m}{\pi^2 \hbar^2 a} \ .$$

Thus,

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

We obtain

$$a^3 U_0 I_3(\epsilon) \leq \frac{m a^2 U_0}{\pi^2 \hbar^2} \ll 1 \ .$$

Thus there is no pole.

(c) **Compare the results with the standard quantum-mechanical expressions.**

The result (1) coincides with the known quantum mechanical result.

2. Fermionic Green's functions

(a) **Express the particle and current densities of a Fermi gas in terms of its single-particle Green's function.**

The Green's function is defined as

$$iG(r_1, t_1, r_2, t_2) = \langle | T \Psi(r_1, t_1) \Psi^\dagger(r_2, t_2) | \rangle \ .$$

The electron density is defined via

$$n(r, t) = \langle | \Psi^\dagger(r, t) \Psi(r, t) | \rangle$$

Thus

$$n(r, t) = -i \lim_{r' \to r, t' \to t+0} G(r, t; r', t') \ .$$

Note, that t' must necessarily be later than t so that the T operator changes the order of Ψ and $\Psi^\dagger$.

The (probability) current density is defined as

$$\vec{j}(r, t) = -\frac{i\hbar}{2m} \langle | \Psi^\dagger(r, t)(\vec{\nabla} \Psi(r, t)) - (\vec{\nabla} \Psi^\dagger(r, t)) \Psi(r, t) | \rangle$$

This corresponds to

$$\vec{j}(r, t) = -\frac{\hbar}{2m} \lim_{r' \to r, t' \to t+0} (\vec{\nabla}_r - \vec{\nabla}_{r'}) \, G(r, t; r', t') \ .$$

(b) **For a free Fermi gas use the expression for the particle density to derive the relation between the density n and the Fermi momentum p_F. Consider the cases of three- and two-dimensional gases.**

We use

$$n(r,t) = -i \lim_{r'\to r, t'\to t+0} G(r,t;r',t') \ .$$

For the free Fermi gas $G(r,t,t',t') = G_0(r-r', t-t')$, thus

$$n = -iG_0(r=0,-\tau)|_{\tau\to+0} \ .$$

We obtain

$$n = -i \int \frac{d^D q}{(2\pi)^D} \int \frac{d\epsilon}{2\pi} e^{i\epsilon\tau} \frac{1}{\epsilon - \left(\frac{\hbar^2 q^2}{2m} - \mu\right) + i0\, \mathrm{sign}\, \epsilon}$$

Since $\tau > 0$ the integral over ϵ should be closed in the upper half-plane. Then the integral gives i only is $\hbar^2 q^2/(2m) - \mu < 0$. We obtain

$$n = \int \frac{d^D q}{(2\pi)^D} \theta\left(\mu - \frac{\hbar^2 q^2}{2m}\right)$$

For $D = 3$ we obtain

$$n = \int_0^{q_F} \frac{q^2 dq}{2\pi^2} = \frac{q_F^3}{6\pi^2} \ ,$$

where $q_F = \sqrt{2mE_F/\hbar^2}$ and $E_F = \mu$. We should also take into account the spin degeneracy, thus $n = 2 \times q_F^3/(6\pi^2)$.

For $D = 2$ we obtain

$$n = \int_0^{q_F} \frac{q dq}{2\pi} = \frac{q_F^2}{4\pi} \ .$$

Taking into account spin $n = 2 \times q_F^2/(4\pi)$.

For $D = 1$ we obtain

$$n = \int_0^{q_F} \frac{dq}{\pi} = \frac{q_F}{\pi} \ .$$

Taking into account spin $n = 2 \times q_F/\pi$.

3. Friedel oscillations

(a) **For free fermions in a one-dimensional space (i.e., moving on a line) find the explicit expression for the Green's function $G_{\alpha\beta}(\epsilon; x, x')$.**

In Fourier representation

$$G_{\alpha\beta}(\epsilon, q) = \frac{\delta_{\alpha\beta}}{\epsilon - \left(\frac{q^2}{2m} - \mu\right) + i0\, \mathrm{sign}\, \epsilon}$$

Then

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

$$G_{\alpha\beta}(\epsilon, x-x') = -\frac{2m}{\hbar^2}\int \frac{dq}{2\pi}\,\frac{\delta_{\alpha\beta}\,e^{iq(x-x')}}{q^2 - \frac{2m}{\hbar^2}(\mu+\epsilon) - i0\,\mathrm{sign}\,\epsilon}\ . \tag{3}$$

It is sufficient to perform the calculation for $x > x'$, since $G(\epsilon, x, x') = G(\epsilon, x', x)$. Then we close the contour of integration over q in the upper half-plane. The possible poles are

$$q_\pm = \pm\sqrt{\frac{2m}{\hbar^2}(\mu+\epsilon) + i0\,\mathrm{sign}\,\epsilon}\ .$$

One of these poles is necessarily in the upper half-plane. For example if $\mu + \epsilon > 0$ and $\epsilon > 0$ it is q_+. Then

$$G_{\alpha\beta}(\epsilon, x-x') = -\frac{im}{\hbar^2}\frac{\delta_{\alpha\beta}\,e^{iq_+|x-x'|}}{q_+}\ .$$

(b) **Repeat the calculation for the half-line $x > 0$ with the hard-wall boundary condition $\psi(x=0) = 0$.**

The easiest way to solve the problem is to realise that the combination

$$G_{hw}(\epsilon, x, x') = G(\epsilon, x, x') - G(\epsilon, x, -x')$$

satisfies the boundary condition. This resembles the image charge method in electrostatics.

Another option is to realise that the exponential factor $e^{iq(x-x')}$ corresponds to the product of two normalised plane waves $(e^{iqx}/\sqrt{L})(e^{iqx'}/\sqrt{L})^*$ (the factors of $1/\sqrt{L}$ are then absorbed by the integration over q). In the new situation the normalised wave functions are $\sqrt{2}\sin(q_n x)/\sqrt{L}$ with $q_n = n\pi/L$ and $n > 0$. Then

$$G_{\alpha\beta}(\epsilon, x-x') = \sum_n \frac{\delta_{\alpha\beta}\,(2/L)\sin(q_n x)\sin(q_n x')}{\epsilon - \left(\frac{\hbar^2 q^2}{2m} - \mu\right) + i0\,\mathrm{sign}\,\epsilon}\ .$$

$$G_{\alpha\beta}(\epsilon, x-x') = \int_0^\infty \frac{2dq}{\pi}\,\frac{\delta_{\alpha\beta}\,\sin(qx)\sin(qx')}{\epsilon - \left(\frac{\hbar^2 q^2}{2m} - \mu\right) + i0\,\mathrm{sign}\,\epsilon}\ .$$

or

$$G_{\alpha\beta}(\epsilon, x-x') = \int_{-\infty}^\infty \frac{dq}{\pi}\,\frac{\delta_{\alpha\beta}\,\sin(qx)\sin(qx')}{\epsilon - \left(\frac{\hbar^2 q^2}{2m} - \mu\right) + i0\,\mathrm{sign}\,\epsilon}\ .$$

This confirms the "image charge" methods.

(c) **In the latter case, show that the fermion density $n(x)$ oscillates as a function of the distance x from the boundary (the so-called Friedel oscillations). What is the period of the oscillations? Plot the resulting density $n(x)$.**

For the density we obtain then

$$n(x) = 2\times\int_0^\infty \frac{2dq}{\pi}\,\theta\left(\mu - \frac{\hbar^2 q^2}{2m}\right)\sin^2(qx)\ .$$

$$n(x) = \frac{4}{\pi}\int_0^{q_F}\sin^2(qx) = \frac{2}{\pi}\left(q_F - \frac{\sin(2q_F x)}{2x}\right)\ .$$