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21.11.2003

Übungen zur Festkörpertheorie I — WS03/04

3. Übungsblatt

1. <u>The free electron Green's function</u>

   Consider the causal or retarded Green's function $G_E(\vec{k})$ of an electron with energy-momentum relation $\varepsilon_{\vec{k}}$,

   $$G_E(\vec{k}) = \frac{1}{E - \varepsilon_{\vec{k}} + i0} ,$$

   where 0 is a positive, infinitesimally small number.

   a) Show by Fourier transforming with respect to E to the time domain, that $G_E(\vec{k})$ obeys causality, i.e. it is non-vanishing only for positive times $t \geq 0$.
   <u>Hint:</u> Use contour integration with respect to the (complex) variable E.

   b) Fourier transform the Green's function in three dimensions to position space and show that

   $$G_E(\vec{r} - \vec{r}') = \frac{e^{iK(E)|\vec{r}-\vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|} \qquad K(E) = \sqrt{2mE/\hbar^2} .$$

2. <u>The Green's function (KKR) method for lattice electrons: boundary conditions</u>
   The single-electron Bloch wave function on a lattice can be obtained in terms of the lattice Green's function $\mathcal{G}_{\vec{k},E(\vec{k})}(\vec{r} - \vec{r}')$, definied in the lecture, as

   $$\Psi_{\vec{k}}(\vec{r}) = \int d^3r' \mathcal{G}_{\vec{k},E(\vec{k})}(\vec{r} - \vec{r}') V(r') \Psi_{\vec{k}}(\vec{r}') , \qquad (*)$$

   where $V(\vec{r}')$ is the atomic core potential, $V(\vec{r}') \neq 0$ only for $|\vec{r}'| < r_0$. This means that $\Psi_{\vec{k}}(\vec{r})$ can be calculated in the complete space, once it is known in the atomic core region, $|\vec{r}'| < r_0$. To obtain the solution for $|\vec{r}'| < r_0$, the boundary conditions at $|\vec{r}'| = r_0$ must be fixed.

   a) Show from the definition of $\mathcal{G}_{\vec{k},E(\vec{k})}(\vec{r} - \vec{r}')$ that in the atomic core region ($|\vec{r}|, |\vec{r}'| < r_0$), the lattice Green's function obeys the same equation of motion as the *free* electron Green's function

   $$\left(E + \frac{\hbar^2\nabla^2}{2m}\right) \mathcal{G}_{\vec{k},E(\vec{k})}(\vec{r} - \vec{r}') = \delta(\vec{r} - \vec{r}') , \qquad |\vec{r}|, |\vec{r}'| < r_0$$

b) Using the Schrödinger equation for $|\vec{r}'| < r_0$, eliminate $V(r')$ from $(*)$ and show that for all $\vec{r}$

$$\int_{r'<r_0} d^3r' \nabla' \cdot \left[\mathcal{G}_{\vec{k},E(\vec{k})}(\vec{r}-\vec{r}')\nabla'\Psi_{\vec{k}}(\vec{r}') - \Psi_{\vec{k}}(\vec{r}')\nabla'\mathcal{G}_{\vec{k},E(\vec{k})}(\vec{r}-\vec{r}') \right] = 0. \quad (**)$$

Hint: Use $\nabla' \cdot [\mathcal{G}\nabla'\Psi - \nabla'\Psi\mathcal{G}] = \mathcal{G}\nabla'^2\Psi - \Psi\nabla'^2\mathcal{G}$.

c) Rewrite $(**)$ as an integral over the surface $r' = r_0$ using Gauß' theorem. Discuss during the exercise session how from this surface boundary condition (valid for *all* $\vec{r}$ on the surface $r = r_0$!) the wave function $\Psi(\vec{r})$ can be determined uniquely in the core region.

3. The degenerate Fermi gas: A model for white dwarfs

One of the possible end states in the life of a very old star is called "white dwarf". In a simple model, it consists of a non-interacting electron gas and an ionic background, which is responsible for ensuring charge neutrality and the compactness of the star by gravitation. The electron density is typically $n = 10^{30}/cm^3$ and the mass of the star $M = 10^{30}kg$. Because of the high density (i.e. high Fermi energy ε_F) a large fraction of the electrons moves relativistically, i.e. we have the energy momentum relation $\varepsilon_p = \sqrt{(mc^2)^2 + c^2p^2}$.

a) Calculate the Fermi momentum p_F of the electron gas in dependence of the electron density. Estimate above which density n the electrons move relativistically, i.e. $p_F > mc$.

b) The temperature of a white dwarf is about $T = 10^7K$. Calculate the Fermi energy ε_F of the electron gas for the electron density given above and show $\varepsilon_F \gg k_BT$. We can therefore calculate at $T = 0$ (!).

c) Calculate the energy E of the electron system depending on the radius R of the star (1) for non-relativistic electrons, $\varepsilon_p = mc^2 + p^2/2m$, and (2) for ultrarelativistic electrons $\varepsilon_p = cp$.

d) Compute the pressure $P = -\partial E/\partial V$ (with V the volume of the star) of the electron system, the so-called Pauli pressure.

e) Now consider the total energy of the star $E_{tot}(R) = E + E_{grav}$, $E_{grav} = -GM^2/R$. Sketch $E(R)$ in a single diagram for small (ultrarelativistic) and for large (non-relativistic) star radius R. What is (qualitatively) the condition on $E(R)$ that there exists a radius R for which the star is stable? Show that above a critical mass M_c the white dwarf cannot be stable. It then undergoes a gravitational collapse. M_c is called the Chandrasekhar mass.