CONTRIBUTION TO THE THEORY OF LOCALIZED PERTURBATIONS IN LARGE SYSTEMS

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We evaluate the energy shift for the ground state of a large Fermi system when a localized perturbation is switched on, taking the interaction between the particles in the system into account. The energy levels of the localized states are then broadened into bands. We establish a condition for the applicability of single-particle approximations to the description of states of this kind.

THE theory of localized perturbations in large Fermi systems (in particular, the theory of defects in crystal lattices) has up to the present time been constructed in the framework of the independent-particle model. It is known, all the same, that the approximation involved in this model is insufficient for a number of problems. Recent progress in the physics of many-particle systems (see, for instance, reference 1 which lists an extensive bibliography) enables us now to approach anew also the problem of localized perturbations, using field-theory methods.

1. THE EVALUATION OF THE SHIFT IN THE GROUND STATE ENERGY

We consider here the problem of the shift in the ground state energy of a large system of interacting fermions when a localized perturbation is adiabatically switched on.

We can write the Hamiltonian of the system in the second quantization representation in the form

$$H = H_0 + \lambda\hat{V}, \tag{1.1}$$

$$\hat{V} = \int dx V(\mathbf{x})\,\psi^+(\mathbf{x})\,\psi(\mathbf{x}); \tag{1.2}$$

H_0 contains the interaction between the fermions, and λ is the parameter which switches on the perturbation. The operators $\psi^+(\mathbf{x})$ and $\psi(\mathbf{x})$ satisfy the well-known commutation relations

$$[\psi(\mathbf{x}), \psi^+(\mathbf{x}')] = \delta(\mathbf{x}-\mathbf{x}'),$$

$$[\psi(\mathbf{x}), \psi(\mathbf{x}')] = [\psi^+(\mathbf{x}), \psi^+(\mathbf{x}')] = 0. \tag{1.3}$$

The energy of the perturbed ground state of the system can be written in the form

$$E = \langle\Psi | H_0 + \lambda\hat{V} | \Psi\rangle, \tag{1.4}$$

where Ψ is the actual state-vector of the system, or

$$E = \langle\Psi | H_0 | \Psi\rangle - i\lambda\int dx V(\mathbf{x}) \lim_{\mathbf{x}'\to\mathbf{x};\,t'\to t+0} G_\lambda(\mathbf{x}, t; \mathbf{x}', t'). \tag{1.5}$$

We have introduced here a single-particle Green's function by the relation (reference 1 gives a bibliography on Green's functions)

$$G_\lambda(x, x') = i\langle\Psi(\lambda)|T(\psi(x)\psi^+(x'))|\Psi(\lambda)\rangle; \tag{1.6}$$

x, x' are points in four-space and T indicates Wick's chronologically ordered product.

We use the obvious consequence of the fact that the ground state energy of the system is stationary with respect to a variation of the state vectors:

$$dE/d\lambda = \langle\Psi(\lambda)|\hat{V}|\Psi(\lambda)\rangle. \tag{1.7}$$

The expression ΔE in which we are interested can then be written as follows:

$$\Delta E = -i\int_0^\lambda d\lambda \int dx V(\mathbf{x}) \lim_{t'\to t+0} G_\lambda(\mathbf{x}, t; \mathbf{x}, t'). \tag{1.8}$$

If we write the Green's function $G_\lambda(\mathbf{x}, t; \mathbf{x}, t')$ as a Fourier integral in the energy ϵ, we get

$$\Delta E = \frac{1}{2\pi i}\int_0^\lambda d\lambda \int dx \lim_{t'\to t+0} \int_C d\varepsilon e^{i\varepsilon(t'-t)} V(\mathbf{x})\, G_\lambda(\mathbf{x}, \mathbf{x}; \varepsilon). \tag{1.9}$$

The choice of the contour C in this equation is connected with some general analytical properties of G_λ. The function G_λ is defined by the following formal operator relation[2]

$$G_\lambda = G\frac{1}{1-\lambda VG}, \tag{1.10}$$

where G is the complete unperturbed fermion Green's function. Its Fourier transform can be written in the form

$$G(\mathbf{k}, \varepsilon) = [\varepsilon - \varepsilon(\mathbf{k}) - M(\mathbf{k}, \varepsilon)]^{-1}. \tag{1.11}$$

Here $M(\mathbf{k}, \epsilon)$ is the irreducible operator of the fermion self-energy. $M(\mathbf{k}, \epsilon)$ has a cut on the

real axis for $-\infty < \epsilon < \epsilon_F$ and $\epsilon_F < \epsilon < \infty$. The branch point ϵ_F is the Fermi energy which is perturbed by the interaction.

The function G_λ has still poles corresponding to localized states with energies $\epsilon < 0$ which satisfy the equation

$$1 - \lambda V G(\varepsilon) = 0. \tag{1.12}$$

One sees easily that these poles lie indeed on the analytical continuation of G_λ in the upper half-plane of complex ϵ. It will, however, become clear in the following that they can be replaced in the discussion by some singular points on the real axis. The integration contour in (1.9) goes thus slightly below the real axis for $-\infty < \epsilon < \epsilon_F$ and slightly above it for $\epsilon_F < \epsilon < \infty$.

The exponential factor in (1.9) makes it possible to apply the residue theorem only in the upper half-plane and can formally be omitted. We have thus

$$\Delta E = \frac{1}{2\pi i}\int^{\lambda} d\lambda \int d\mathbf{x} \int_C d\varepsilon V(\mathbf{x})\, G(\mathbf{x}, \mathbf{x}'; \varepsilon) \frac{1}{1 - \lambda V(\mathbf{x}')\, G(\mathbf{x}', \mathbf{x}; \varepsilon)}. \tag{1.13}$$

Integrating over λ we have

$$\Delta E = -\frac{1}{2\pi i}\int_C d\varepsilon \,\mathrm{Sp}\ln(1 - \lambda V G(\varepsilon)). \tag{1.14}$$

This last equation can be written in the form[2]

$$\Delta E = -\frac{1}{2\pi i}\int_C d\varepsilon \ln\det(1 - \lambda V G(\varepsilon)). \tag{1.15}$$

We consider now the imaginary part of the integrand in (1.15). Under quite general assumptions[2] about the character of the perturbation we have

$$\mathrm{Im}\ln\det(1 - \lambda V G(\varepsilon)) = \mathrm{arc\,tg}\frac{-\lambda V \,\mathrm{Im}\, G(\varepsilon)}{1 - \lambda V \,\mathrm{Re}\, G(\varepsilon)}. \tag{1.16}*$$

Here

$$\mathrm{Im}\, G(\mathbf{x}, \varepsilon) = (2\pi)^{-3}\int d\mathbf{k} e^{i\mathbf{k}\mathbf{x}} \frac{-\mathrm{Im}\, M(\mathbf{k}, \varepsilon)}{(\varepsilon - \varepsilon(\mathbf{k}) - \mathrm{Re}\, M(\mathbf{k}, \varepsilon))^2 + (\mathrm{Im}\, M(\mathbf{k}, \varepsilon))^2} \times [\eta(\mathbf{k} - \mathbf{k}_F) - \eta(\mathbf{k}_F - \mathbf{k})], \tag{1.17a}$$

$$\mathrm{Re}\, G(\mathbf{x}, \varepsilon) = (2\pi)^{-3}\int d\mathbf{k} e^{i\mathbf{k}\mathbf{x}} \frac{\varepsilon - \varepsilon(\mathbf{k}) - \mathrm{Re}\, M(\mathbf{k}, \varepsilon)}{(\varepsilon - \varepsilon(\mathbf{k}) - \mathrm{Re}\, M(\mathbf{k}, \varepsilon))^2 + (\mathrm{Im}\, M(\mathbf{k}, \varepsilon))^2}. \tag{1.17b}$$

We shall see in the following that when $\epsilon < 0$, $\mathrm{Im}\, G(\epsilon)$ is small and decreases rather fast with increasing $|\epsilon|$. Neglecting therefore $(\mathrm{Im}\, G(\epsilon))'$ in comparison with $\mathrm{Im}\, G(\epsilon)$ we find

$$\frac{d}{d\varepsilon}\arg\det(1 - \lambda V G(\varepsilon)) = -\frac{\lambda V \,\mathrm{Im}\, G(\varepsilon)\,(d/d\varepsilon)[\lambda V \,\mathrm{Re}\, G(\varepsilon)]}{(1 - \lambda V \,\mathrm{Re}\, G(\varepsilon))^2 + (\lambda V \,\mathrm{Im}\, G(\varepsilon))^2} \equiv f(\varepsilon). \tag{1.18}$$

*arctg = $\tan^{-1}$

We go now over to the limit $\mathrm{Im}\, G(\epsilon) \to 0$:

$$\lim_{\mathrm{Im}\, G(\varepsilon)\to 0} \frac{d}{d\varepsilon}\arg\det(1 - \lambda V G(\varepsilon)) = \pi\sum_i \delta(\varepsilon - \varepsilon'_{0i}). \tag{1.19}$$

In this equation ϵ'_{0i} are the energies of the "physical" localized states which are determined from the equation

$$1 - \lambda V \,\mathrm{Re}\, G(\varepsilon'_{0i}) = 0 \qquad (\varepsilon'_{0i} < 0). \tag{1.20}$$

We have thus

$$\int_{-\infty}^{0} \lim_{\mathrm{Im}\, G(\varepsilon)\to 0} \frac{d}{d\varepsilon}\arg\det(1 - \lambda V G(\varepsilon))\, d\varepsilon = \nu\pi, \tag{1.21}$$

where ν is the total number of localized states.

In the case where $\mathrm{Im}\, G(\epsilon) \neq 0$, ν can be written in the form

$$\nu = \frac{1}{\pi}\int_{-\infty}^{0} f(\varepsilon)\, d\varepsilon. \tag{1.22}$$

In our discussion there enters thus naturally the energy distribution function $f(\epsilon)$ of the localized states which is given by (1.18). This function has a steep maximum near each of the roots of (1.20).

We turn now to the evaluation of ΔE and we take into account that we can assume $\ln\det(1 - \lambda V G(\epsilon))$ to be a regular function on its Riemann surface in the upper half-plane and it can then under well-known limitations imposed upon V (see references 2 and 3) on the real axis be expressed in terms of its imaginary part, as follows[3]

$$\ln\det(1 - \lambda V G(\varepsilon)) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\arg\det(1 - \lambda V G(\varepsilon'))}{\varepsilon - \varepsilon'} d\varepsilon'. \tag{1.23}$$

After taking residues in the expression for ΔE we integrate the contribution from the "discrete" states by parts which leads to

$$\Delta E = \frac{1}{\pi}\int_{-\infty}^{0} \varepsilon f(\varepsilon)\, d\varepsilon - \frac{1}{\pi}\int_{0}^{\varepsilon_F} \arg\det(1 - \lambda V G(\varepsilon))\, d\varepsilon. \tag{1.24}$$

This reminds us of the relation derived by I. M. Lifshitz,[4] but there is an essential difference in the first term which is connected with the localized states and this compels us to revise the concept itself of states of this kind. These are not ordinary discrete states but are wave packets where states with arbitrary ϵ from the interval $-\infty < \epsilon < 0$ are present with weights proportional to $f(\epsilon)$. Each ("physical") discrete level is broadened into a band. Different states in the band are occupied with a probability proportional to $f(\epsilon)$. One sees easily that the effective width of this band is given by the imaginary part of the root of Eq. (1.12) when it is analytically continued in the upper ϵ-half-plane.

2. THE WIDTH OF THE LEVELS OF THE LOCALIZED STATES

The analytical continuation mentioned a moment ago is easily obtained if we consider $G_+(\epsilon)$ and $G_-(\epsilon)$. The function $G_+(\epsilon)$ corresponds to $G(\epsilon)$ of section 1 while the integration contour for $G_-(\epsilon)$ is above the real axis for $e < e_F$ and below it for $\epsilon > \epsilon_F$. Because the Hamiltonian is Hermitian we have on the real axis $G_+(\epsilon) = \overline{G}_-(\epsilon)$.

We now expand $G_+(\epsilon)$ around $\epsilon'_{0i} - i\delta(\delta > 0)$. We get for the imaginary part of the root of (1.12)

$$\frac{1}{2}\Gamma(\varepsilon_0) = V \operatorname{Im} G(\varepsilon_0) \Big/ \left[\frac{d}{d\varepsilon} V \operatorname{Re} G(\varepsilon)\right]_{\varepsilon=\varepsilon_0} \quad (2.1)$$

For the sake of simplicity we write in the following ϵ_0 instead of ϵ'_{0i} and $G(\epsilon_0)$ instead of $G_+(\epsilon_0)$.

We now bear in mind that for $\epsilon < 0$ we have $\operatorname{Im} G_0(\epsilon) = 0$ and thus

$$\operatorname{Im} G(\varepsilon) = \operatorname{Re} G_0(\varepsilon) \operatorname{Im} \frac{1}{1 - MG_0(\varepsilon)}, \quad (2.2)$$

where $G_0(\epsilon)$ is the Green's function when there are no interactions.

When we take into account that $\operatorname{Re} G_0(\epsilon)$ decreases when $|\epsilon|$ increases we can find for sufficiently large $|\epsilon_0|$

$$\Gamma(\varepsilon_0) = 2V \operatorname{Re} G_0(\varepsilon_0) \operatorname{Im} M \operatorname{Re} G_0(\varepsilon_0) \Big/ \left[\frac{d}{d\varepsilon} V \operatorname{Re} G_0(\varepsilon)\right]_{\varepsilon=\varepsilon_0} \quad (2.3)$$

This equation can be rewritten as follows (if we use the explicit form of $G_0(\epsilon)$ and assume that V does not introduce any analytical complications)

$$\Gamma(\varepsilon_0) = 2V \operatorname{Re} G_0(\varepsilon_0) \operatorname{Im} M \operatorname{Re} G_0(\varepsilon_0) / V (\operatorname{Re} G_0(\varepsilon_0))^2. \quad (2.4)$$

We shall now consider the important case of a model with a δ-function perturbation when V = constant in the k-representation. In that case

$$\Gamma(\varepsilon_0) = 2 \int \operatorname{Im} M(\mathbf{k}, \varepsilon_0) \times (\operatorname{Re} G_0(\mathbf{k}, \varepsilon_0))^2 d\mathbf{k} \Big/ \int (\operatorname{Re} G_0(\mathbf{k}, \varepsilon_0))^2 d\mathbf{k} \quad (2.5)$$

and Γ depends thus on the perturbation only through ϵ_0.

For our further considerations we need to know the asymptotic behavior of $\operatorname{Im} M(\mathbf{k}, \epsilon_0)$ for large negative ϵ_0. To get this we write down an explicit expression in the simplest approximation[5]

$$\operatorname{Im} M(\mathbf{k}, \varepsilon_0) = -\frac{\xi}{4\pi} \int \frac{d\mathbf{q}}{q^2} \frac{\operatorname{Im} P(\mathbf{q}, \Delta\varepsilon)}{|1 - P(\mathbf{q}, \Delta\varepsilon)|^2} \eta(|\mathbf{k} - \mathbf{q}| - 1), \quad (2.6)$$

where

$$\Delta\varepsilon = \varepsilon(\mathbf{k} - \mathbf{q}) - \varepsilon_0, \quad (2.7)$$

$P(\mathbf{q}, \Delta\epsilon)$ is the polarization operator and $\xi = e^2 k_F / \pi e_F$. In our case $\Delta\epsilon$ is large and as $P(\mathbf{q}, \Delta\epsilon)$ is then small we have

$$\operatorname{Im} M(\mathbf{k}, \varepsilon_0) = -\frac{\xi}{4\pi} \int \frac{d\mathbf{q}}{q^2} \operatorname{Im} P(\mathbf{q}, \Delta\varepsilon) \eta(|\mathbf{k} - \mathbf{q}| - 1). \quad (2.8)$$

We restrict ourselves to the lowest order polarization operator $P_0(\mathbf{q}, \Delta\epsilon)$. The quantity $P_0(\mathbf{q}, \Delta\epsilon)$ is for sufficiently large $\Delta\epsilon$ different from zero only in the interval

$$-1 + \sqrt{1 + \Delta\varepsilon/\varepsilon_F} \leqslant q/q_F \leqslant 1 + \sqrt{1 + \Delta\varepsilon/\varepsilon_F} \quad (2.9)$$

and can be written in dimensionless units ($y = \Delta\epsilon/\epsilon_F$, $x = q/q_F$) as follows[6]

$$\operatorname{Im} P_0(x, y) = -\frac{\pi\xi}{2x^3}\left[1 - \frac{1}{4}\left(\frac{y}{x} - x\right)^2\right]. \quad (2.10)$$

This enables us to evaluate the average value of the integral in (2.8) by putting

$$\Delta x = 2, \qquad x = \sqrt{y}. \quad (2.11)$$

We note now that by virtue of (2.7)

$$y = x^2 + \Delta - \mathbf{kq}/\varepsilon_F, \qquad \Delta = [\varepsilon(\mathbf{k}) - \varepsilon_0]/\varepsilon_F. \quad (2.12)$$

The main contribution to (2.8) is thus provided by those values of q which satisfy the relation

$$\mathbf{kq}/\varepsilon_F = \Delta. \quad (2.13)$$

This gives

$$\operatorname{Im} P_0(x, y) = -\frac{\pi\xi}{2x^3}. \quad (2.14)$$

In this equation x is determined from (2.13).

The remaining integration over the angle (from 0 to $\pi/2$, as $\Delta > 0$) is trivial. If $|\epsilon_0| > e_F$ we get

$$\operatorname{Im} M(k, \varepsilon_0) = 4\pi\varepsilon_F \xi^2 (k/k^F)^3 \Delta^{-3}. \quad (2.15)$$

We can now find $\Gamma(\epsilon_0)$ from (2.5):

$$\Gamma(\varepsilon_0) = \frac{\sqrt{2}}{3} \varepsilon_F \xi^2 \left(\frac{|\varepsilon_0|}{\varepsilon_F}\right)^{-3/2} \quad (2.16)$$

The single-particle approximation gives only a real contribution to $M(\mathbf{k}, \epsilon_0)$. It is thus possible for us to establish some criterion for the applicability of the independent particle model to a description of localized states. This can be written in the form

$$\xi^2 \left(\frac{|\varepsilon_0|}{\varepsilon_F}\right)^{-3/2} \ll 1. \quad (2.17)$$

It follows from general considerations that contributions in higher order perturbation theory to $\Gamma(\epsilon_0)$ decrease faster than the term (2.16) and this determines how effective the criterion (2.17) will be. Condition (2.17) is for the case of lattice defects rather well satisfied and this justifies to a certain extent the application of single-electron theories to describe defects.

It is necessary to note in conclusion that we have practically made no use of perturbation theory as far as V is concerned. Such a theory must be constructed rather carefully to avoid divergences which are possible when localized states are formed. Schwinger[2,3] has considered a similar problem.

[1] The collection: Вопросы квантовой теории многих тел (Problems in the Quantum Theory of Many-Body Systems) IIL, 1959.

[2] J. Schwinger, Phys. Rev. **93**, 615 (1954).

[3] J. Schwinger, Phys. Rev. **94**, 1362 (1954).

[4] I. M. Lifshitz, Usp. Mat. Nauk **7**, 171 (1952).

[5] D. F. Dubois, Doctoral Thesis, California Institute of Technology, 1959.

[6] J. Hubbard, Proc. Roy. Soc. (London) **A243**, 336 (1958).

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