THE FERMI SURFACE FOR POINT INTERACTIONS

Raphael Høegh-Krohn

Helge Holden

Steinar Johannesen

Tore Wentzel-Larsen

Matematisk institutt

Universitetet i Oslo

Blindern, Oslo 3

Norge

Abstract:

Using a computer we study the Fermi surface for the one electron model of an infinite crystal in three dimensions with zero range interactions, i.e. with so-called point interactions.

A computer program is available which has as input the crystal structure, the scattering length of the solid considered and the Fermi energy and as output a drawing of the corresponding Fermi surface inside its Brillouin zone.

1. Introduction.

The notion of Fermi surface is of great importance in solid state physics, and let us first recall what we mean by a Fermi surface.

In the one electron model of an infinite three dimensional crystal we consider the Schrödinger operator $H = -\Delta + V$ (in units where $\hbar = 1$, $m = \frac{1}{2}$) on $L^2(\mathbb{R}^3)$ where Δ is the Laplacian and V is periodic with periodicity Λ where Λ is a three dimensional lattice in $\mathbb{R}^3$. By standard techniques this implies that

$$H = \int_{\hat{\Lambda}}^{\oplus} H(k) d^3k$$

where the dual group $\hat{\Lambda} = \mathbb{R}^3/\Gamma$ can be identified with the Brillouin zone B , i.e. a Wigner-Seitz cell of the orthogonal (or dual) lattice Γ .

The band spectrum of H dissolves into discrete eigenvalues $E_1(k) \leq E_2(k) \leq \dots$ of $H(k)$ and the Fermi surface is the set $\{k \in B \mid E_n(k) = E_F \text{ for a } n \in \mathbb{N}\}$ where E_F is the Fermi energy which distinguish the occupied states from the nonoccupied ones at zero temperature in the Fermi-Dirac statistics.

Instead of considering the Fermi surface inside the Brillouin zone B , one can consider it on $\mathbb{R}^3$ by extending it periodically.

The actual computation of the Fermi surface is a mixture of theory and experiment with no unifying rigorous theory. See [1] for an extensive introduction to the subject. Actually it seems that the only Fermi surface that has been computed explicitly starting with an explicit potential is the free electron approximation, i.e. with no interaction.

In this paper we compute with the aid of a computer the

Fermi surface explicitly starting from a non-trivial interaction, namely point interaction.

The study of Schrödinger operators with point interactions, i.e. zero range interactions or Fermi pseudo-potentials, was started by among others Fermi, Peierls, Breit, Thomas in the thirties in nuclear physics [2], and continued in the fifties by Huang, Yang, Lee, Luttinger and others in statistical mechanics [3].

In addition, and in this connection more interesting, we have the celebrated Kronig-Penney model [4], dating from 1933, which is a model of an infinite one-dimensional crystal with point interactions.

The non-trivial rigorous study of these operators especially in three dimensions was started in 1961 by Berezin, Faddeev and others [5] and made into a systematic theory by Grossmann, Høegh-Krohn and Mebkhout [6], [7]. In particular, in [7] the periodic point interaction model is constructed, and its spectral properties are determined.

Thus the model we study here is a three dimensional analogue of the Kronig-Penney model.

More detailed properties of the spectrum when one removes some points with point interaction and thus destroys the periodicity are studied in [11].

Starting off from this there has been a thorough rigorous study of these operators and related operators with more realistic short-range potential. For an extensive exposition of all this we refer to [12].

We also note en passant that in the beginning of this rigorous study non-standard analysis played an important part [8].

One property of the point interactions is that the only parameter needed to specify the interaction completely is the scattering length.

Thus the equation we derive for the Fermi surface contains only the scattering length of the one center problem, the Fermi energy and the lattice.

This implies that the computer program [14] has as input the lattice, the scattering length and the energy and as output the Fermi surface with the following four options:

- (i) The surface within the corresponding Brillouin zone.
- (ii) The surface over an arbitrary rectangle in the plane.
- (iii) Contour maps of (i).
- (iv) Contour maps of (ii).

The Fermi surface is mathematically a multivalued, actually infinitely valued, function.

The computer program is however only able to draw single-valued functions, so we can only see half the surface in (i) and a single sheet in (ii). In this short paper we can only give some examples of Fermi surfaces for a small number of different lattices and values of the parameters.

However a specific Fermi surface with a particular lattice and values of the parameters can be obtained from the authors on request.

One may argue that a point interaction is not a realistic interaction. However one virtue of the point interaction is that one can actually compute a non-trivial Fermi surface starting from a potential. In addition it is a possible starting point for a more general approach.

Namely we can show [9] (see next section) that the Schrödinger operator with point interactions is very well approximated (actually in norm resolvent sense) by Schrödinger operators with more general short range interactions. We will return to this in connection with Fermi surfaces later.

2. Point interactions and Fermi surfaces.

We study here the one-electron model of an infinite crystal in three dimensions with point interactions.

More precisely, let Λ be a Bravais lattice in $\mathbb{R}^3$, i.e.

$$\Lambda = \{n_1 a_1 + n_2 a_2 + n_3 a_3 \mid n_i \in \mathbb{Z}\} \quad (1)$$

where $a_1, a_2, a_3 \in \mathbb{R}^3$ are three independent vectors. We consider here the case where we have exactly one atom for each Bravais lattice point.

The Schrödinger operator $-\Delta_\alpha$ corresponding to point interactions with strength α at each point in Λ has resolvent with integral kernel:

$$\begin{aligned} (-\Delta_\alpha - E)^{-1}(p, q) = & \quad (2) \\ (p^2 - E)^{-1} \delta(p - q) + (2\pi)^{-3} \sum_{\lambda, \lambda' \in \Lambda} \left[\left(\alpha - \frac{i\sqrt{E}}{4\pi} \right) \delta_{\lambda\lambda'} - \tilde{G}_E(\lambda - \lambda') \right]_{\lambda\lambda'}^{-1} \frac{e^{i(p\lambda - q\lambda')}}{(p^2 - E)(q^2 - E)} \end{aligned}$$

where $\text{Im}\sqrt{E} > 0$ and

$$\tilde{G}_E(x) = \begin{cases} \frac{e^{i\sqrt{E}|x|}}{4\pi|x|} & x \neq 0 \\ 0 & x = 0 \end{cases} \quad (3)$$

(Recall that $\frac{e^{i\sqrt{E}|x-y|}}{4\pi|x-y|}$ is the integral kernel of $(-\Delta - E)^{-1}$ on $L^2(\mathbb{R}^3)$) and $[]_{\lambda\lambda'}^{-1}$ denotes the (λ, λ') -th element of the

inverse of the matrix $[\]$ on $\ell^2(\Lambda)$.

We briefly digress here to give some insight into the definition of H_α . Formally we are interested in the operator

$$H = -\Delta - \sum_{\lambda \in \Lambda} v \delta(\cdot - \lambda) \quad (4)$$

where δ is Dirac's delta function and $v > 0$ which is not a well-defined self-adjoint operator on $L^2(\mathbb{R}^3)$.

By making a Fourier-transform we obtain the operator

$$H = p^2 - \sum_{\lambda \in \Lambda} v |\phi_\lambda\rangle \langle \phi_\lambda| \quad (5)$$

where

$$\phi_\lambda(p) = (2\pi)^{-3/2} e^{ip\lambda} \quad (6)$$

and the operator $S = |f\rangle\langle g|$ is defined to be $Sh = f(g, h)$, ((g, h) is the inner product on $L^2(\mathbb{R}^3)$) and p^2 is considered as multiplication operator, i.e. $H_0 = p^2$ means $(H_0 f)(p) = p^2 f(p)$.

To make this operator well-defined we modify H in the following way: Replace ϕ_λ with ϕ_λ^ω where

$$\phi_\lambda^\omega(p) = \chi_\omega(p) \phi_\lambda(p) \quad (7)$$

where χ_ω is the characteristic function of a ball with radius ω , i.e.

$$\chi_\omega(p) = \begin{cases} 1 & |p| \leq \omega \\ 0 & |p| > \omega \end{cases} \quad (8)$$

and let v be ω -depending, $v = v(\omega)$.

By choosing

$$v(\omega) = \left(\frac{\omega}{2\pi} + \alpha \right)^{-1} \quad (9)$$

where $\alpha \in \mathbb{R}$ is arbitrary one can show that H^ω where

$$H^\omega = p^2 - v(\omega) \sum_{\lambda \in \Lambda} |\phi_\lambda^\omega\rangle \langle \phi_\lambda^\omega| \quad (10)$$

will converge in strong resolvent sense as $\omega \rightarrow \infty$ to the operator $-\Delta_\alpha$. Note that the coupling constant $v(\omega)$ tends to zero as $\omega \rightarrow \infty$. For more details see [6], [7], [12].

The constant α can be interpreted as related to the scattering length in the sense that $a = 1/4\pi\alpha$ is the scattering length of the one particle system with a single point interaction.

We now return to the operator $-\Delta_\alpha$. Using the invariance under Λ we can write

$$-\Delta_\alpha = \int_{\hat{\Lambda}} -\Delta_\alpha(k) d^3k \quad (11)$$

where the dual group $\hat{\Lambda} = \mathbb{R}^3/\Gamma$ (Γ is the orthogonal lattice, i.e. $\Gamma = \{n_1 b_1 + n_2 b_2 + n_3 b_3 | n_i \in \mathbb{Z}\}$ where $a_i \cdot b_i = 2\pi \delta_{ij}$) can be identified with the Wigner-Seitz cell of the orthogonal lattice, i.e. the Brillouin zone B and where $-\Delta_\alpha(k)$ is a self-adjoint operator on $\ell^2(\Gamma)$ with integral kernel

$$(-\Delta_\alpha(k) - E)^{-1}_{(\gamma, \gamma')} = \quad (12)$$

$$(|\gamma+k|^2 - E)^{-1} \delta_{\gamma\gamma'} + (2\pi)^{-3} \left(\alpha - \frac{i\sqrt{E}}{4\pi} - g_E(k) \right)^{-1} \frac{1}{(|\gamma+k|^2 - E)(|\gamma'+k|^2 - E)}$$

where $\text{Im}\sqrt{E} > 0$ and

$$g_E(k) = \sum_{\lambda \in \Lambda} \tilde{G}_E(\lambda) e^{-i\lambda \cdot k} \quad (13)$$

See [7] for more details.

We see from (12) that the negative part of the spectrum of $-\Delta_\alpha(k)$ consists of points where $\alpha - \frac{i\sqrt{E}}{4\pi} - g_E(k) = 0$.

Using this one can [7] explicitly compute the spectrum of

$-\Delta_\alpha$:

$$\sigma(-\Delta_\alpha) = [E_0(\alpha), E_1(\alpha)] \cup [0, \infty) \quad (14)$$

where $E_1(\alpha) < 0$ provided $\alpha < \alpha_0 < 0$ where α_0 is a suitable constant. $E_0(\alpha), E_1(\alpha)$ will also depend on the lattice.

The equation for the Fermi surface is then

$$\sum_{\lambda \in \Lambda} \tilde{G}_E(\lambda) e^{-i\lambda \cdot k} = \alpha - \frac{i\sqrt{E}}{4\pi} \quad (15)$$

where Λ, α, E are input and the implicit function in k is output and we recall that

$$\tilde{G}_E(\lambda) = \begin{cases} \frac{e^{i\sqrt{E}|\lambda|}}{4\pi|\lambda|} & \lambda \neq 0 \\ 0 & \lambda = 0 \end{cases} \quad (16)$$

When we let $E < 0$ (15) can be written:

$$\sum_{\substack{\lambda \in \Lambda \\ \lambda \neq 0}} \frac{e^{-\sqrt{|E|}|\lambda|}}{|\lambda|} \cos k \cdot \lambda = 4\pi\alpha - \sqrt{|E|}. \quad (17)$$

A few words may be appropriate here to indicate how we solve this equation.

We sum all the terms in the infinite series with $|\lambda| < R$ for some fixed R , use the symmetry of the lattice (which implies that the program works for all Bravais lattices except for triclinic) to simplify and obtain a polynomial equation which can be solved by standard techniques.

In general a n 'th degree equation has n solutions. However, adding more and more terms in (17) which increases the degree of the equation will not yield more and more different solutions which is reasonable since the equation (17) with a

finite sum converges exponentially to the equation for a unique Fermi surface.

But as the computer only is able to draw single valued functions, we usually end up with a small number of different drawings corresponding to different roots of the equation. To visualize the Fermi surface one has to superimpose visually the different drawings.

For example in fig. 1 we use an approximation which yields a third degree equation, and we obtain three drawings which however all are identical to the one in fig. 1.

However in fig. 2 we see an approximation which gives rise to a sixth degree equation, and we obtain six drawings. In this case there are only two with major differences namely fig. 2a and 2b.

In the next section we present some examples of Fermi surfaces with various values of the parameters and for some lattices.

As mentioned in the introduction, point interactions represents a first approximation to more realistic short-range interactions.

To be precise, let

$$H_{\epsilon} = -\Delta + \epsilon^{-2} \mu(\epsilon) \sum_{\lambda \in \Lambda} V((\cdot - \lambda)/\epsilon) \quad (18)$$

where V is a real-valued potential which is Rollnik (i.e.

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} |V(x)V(y)| |x-y|^{-2} dx dy < \infty) \text{ with compact support and } \mu(\epsilon)$$

is an analytic function with $\mu(0) = 1$.

We assume that $-\Delta + V$ has a simple zero-energy resonance, i.e. the equation

$$(-\Delta+V)\phi = 0 \quad (19)$$

has a simple solution ϕ which does not belong to $L^2(\underline{\mathbb{R}}^3)$. To be more specific, using the standard decomposition ($E < 0$)

$$(-\Delta+V-E)^{-1} = G_E - G_E v (1 + u G_E v)^{-1} u G_E \quad (20)$$

where

$$G_E = (-\Delta - E)^{-1} \quad (21)$$

and

$$u = |V|^{\frac{1}{2}} \text{sgn } V; \quad v = |V|^{\frac{1}{2}} \quad (22)$$

we see that eigenvalues of $-\Delta+V$ corresponds to non-trivial solutions of

$$\phi + u G_E v \phi = 0. \quad (23)$$

One can show, see [10], that if ϕ is a solution of (23) then

$$\psi = G_E v \phi \quad (24)$$

is a solution of

$$(-\Delta+V)\psi = E\psi. \quad (25)$$

So we assume that

$$\phi + u G_0 v \phi = 0 \quad (26)$$

has a simple non-trivial solution $\phi \in L^2(\underline{\mathbb{R}}^3)$. Then one can still prove that

$$\psi = G_0 v \phi \quad (27)$$

is a solution of

$$(-\Delta+V)\psi = 0 \quad (28)$$

now in the sense of distributions, and what we assume is that this ψ is not in $L^2(\underline{\mathbb{R}}^3)$.

From this assumption we can prove

Theorem 1.

The operator H_ϵ converges in norm resolvent sense to the operator $-\Delta_\alpha$ given by (2) where α is given according to

$$\alpha = \mu'(0)(V\psi, \psi) | (V, \psi) |^{-2}. \quad (29)$$

Remark: The ψ in the definition of α is the ψ given by (27).

Proof: See [9].

Using the the same decomposition for H_ϵ as for $-\Delta_\alpha$, i.e.

$$H_\epsilon = \int_{\hat{\Lambda}}^{\oplus} H_\epsilon(k) d^3k \quad (30)$$

we dissolve the bands of the spectrum into discrete eigenvalues.

We can then prove the following result.

Theorem 2.

Let $E_0 < 0$ be an eigenvalue of $-\Delta_\alpha(k)$. Then there exists an eigenvalue E_ϵ for $H_\epsilon(k)$ such that $E_\epsilon \rightarrow E_0$ when $\epsilon \rightarrow 0$ and E_ϵ is analytic in ϵ . We have the following expansion

$$E_\epsilon = E_0 + \epsilon E' + o(\epsilon) \quad (31)$$

where

$$E' = h_\Lambda^k (A + E_0 B) \quad (32)$$

and

$$h_\Lambda^k = (2\pi)^3 [|B| \sum_{\gamma \in \Gamma} \frac{1}{(|\gamma + k|^2 - E)^2}]^{-1}. \quad (33)$$

($|B|$ is the Lebesgue measure of the Brillouin zone) and A, B are constants only depending on properties of $-\Delta + V$.

Remark: The explicit form of A and B are given in [9].

Proof: See [9].

Remark: This means that the Fermi surface computed with point interactions represents a first approximation to a Fermi surface with more general short-range interactions.

Using a scaling technique point interactions can also be related to another limit than the zero range limit.

Namely, let

$$H(\varepsilon) = -\Delta + \mu(\varepsilon) \sum_{\lambda \in \Lambda} V(\cdot - \lambda/\varepsilon) \quad (34)$$

where V and μ are as before. Then, using the unitary operator U_ε defined by

$$(U_\varepsilon f)(x) = \varepsilon^{-3/2} f(x/\varepsilon) \quad (35)$$

we see that

$$U_\varepsilon^{-1} H_\varepsilon U_\varepsilon = \varepsilon^{-2} H(\varepsilon) \quad (36)$$

which implies that the eigenvalues E_ε and $E(\varepsilon)$ of H_ε and $H(\varepsilon)$ respectively are related by

$$E_\varepsilon = \varepsilon^{-2} E(\varepsilon). \quad (37)$$

Looking at the operator $H(\varepsilon)$, we see that the limit $\varepsilon \rightarrow 0$ represents a situation where the centers (i.e. the points where each potential $V(x - \lambda/\varepsilon)$, $\lambda \in \Lambda$, is concentrated) move apart. As usual we decompose $H(\varepsilon)$, i.e.,

$$H(\varepsilon) = \bigoplus_{\lambda \in \Lambda} \int H(\varepsilon, k) d^3 k \quad (38)$$

and we have the following theorem

Theorem 3.

Let $E(\varepsilon, k) < 0$ be an eigenvalue of $H(\varepsilon, k)$ such that

$$\lim_{\varepsilon \rightarrow 0} \varepsilon^{-2} E(\varepsilon, k) < 0. \quad (39)$$

Then $E(\varepsilon, k)$ is analytic and has the following expansion

$$E(\varepsilon, k) = \varepsilon^2 E_0 + \varepsilon^3 E' + o(\varepsilon^3) \quad (40)$$

where E_0 is an eigenvalue of $-\Delta_\alpha(k)$ and E' is given by (32).

3. Some Fermi surfaces.

Figure captions.

Fig. 1: The simplest Fermi surface we include here is for a simple cubic crystal (SC or cubic P) with $E = -1$ and $\alpha = 0.12$ and $a = b = c = 1$ (for notation concerning the lattices, see Kittel [13]) inside the upper half of its Brillouin zone. Completely vertical or horizontal parts of the illustration are not parts of the Fermi surface.

Fig. 2a, 2b. The Fermi surface of a body centered crystal (BBC or cubic I) with $E = -1$ and $\alpha = -0.14$ inside the upper half of its Brillouin zone. The total surface within the upper half of the Brillouin zone is the union of the two surfaces depicted above.

Fig. 3a, 3b: A contour plot of fig. 2a, 2b.

Fig. 4a, 4b: The Fermi surface of fig 2a, 2b extended periodically. Again it is difficult to visualize the total surface in the sense that the total Fermi surface is the union of the two surfaces above extended periodically in the positive and negative z-direction.

Fig. 5a, 5b: A contour plot of fig 4a, 4b.

Fig. 6a, 6b: A magnification of part of the surface in fig. 4a, 4

Fig. 7a, 7b: A magnification of another part of the surface in fig. 4a, 4b.

Fig. 8a, b: The Fermi surface of a face centered cubic (FCC or cubic F) crystal with $E = -1$, $\alpha = -0.17$ inside the upper half of the Brillouin zone.

Fig. 9a, b. Contour plot of fig. 8a, b.

Fig. 10a, b: The Fermi surface of fig. 8 extended periodically.

Fig. 11a, b: Contour plot of fig. 10.

Fig. 12a, b: A magnification of a part of fig. 10a, b.

The next seven figures show how the Fermi surface inside the upper half of its Brillouin zone varies with E for an orthorhombic P crystal with axes $a = 3$, $b = 2$, $c = 1$ and with $\alpha = 0$.

Fig. 13: $E = -1.2$. The Fermi surface is homeomorphic to a sphere around each point of the orthogonal lattice.

Fig. 14. $E = -1.1$

Fig. 15. $E = -0.9$. The Fermi surface is now connected in the x-direction.

Fig. 16. $E = -0.425$

Fig. 17. $E = -0.35$. The Fermi surface is connected in the x- and y-directions.

Fig. 18. $E = -0.13$

Fig. 19. $E = -0.1$

The next three figures show a similar series for a tetragonal P crystal with axes $a = b = 2$, $c = 1$ and with $\alpha = 0$.

Fig. 20. $E = -1.1$

Fig. 21. $E = -0.6$

Fig. 22. $E = -0.4$

The next two figures show the Fermi surface inside the upper half of its Brillouin zone for a tetragonal P crystal with axes $a = b = 2$, $c = 3$ and with $\alpha = 0$ for two values of E .

Fig. 23. $E = -0.2417$

Fig. 24. $E = -0.2$. The Fermi surface is now connected in the z-direction.

Fig. 25. The surface for a monoclinic C crystal with axes $a = 2$, $b = 1.5$, $c = 1$ inside the upper half of its Brillouin zone. The angle between the axes $\vec{a}$ and $\vec{c}$ is 60° , $\alpha = 0$ and $E = -1$.

Fig. 26, 27. The Fermi surfaces of a trigonal crystal with $\alpha = 0$ and $E = -1$ for two different angles, 30° and 70° , between the symmetry axis and each of the crystal axes.

Fig. 1

Fig. 2a

Fig. 2b

Fig. 3a

Fig. 3b

Fig. 4a

Fig. 4b

Fig. 5a

Fig. 5b

Fig. 6a

Fig. 6b

Fig. 7a

Fig. 7b

Fig. 8a

Fig. 8b

Fig. 9a

Fig. 9b

Fig. 10a

Fig. 10b

Fig. 11a

Fig. 11b

Fig. 12a

Fig. 12b

Fig. 13

Fig. 14

Fig. 15

Fig. 16

Fig. 17

Fig. 18

Fig. 19

Fig. 20

Fig. 21

Fig. 22

Fig. 23

Fig. 24

Fig. 25

Fig. 26

Fig. 27

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