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# FRIEDEL OSCILLATIONS FROM THE WIGNER-KIRKWOOD DISTRIBUTION IN HALF INFINITE MATTER


Mireille DURAND, Peter SCHUCK

Institut des Sciences Nucléaires, 53, Avenue des Martyrs
38026 Grenoble-Cédex, France

Xavier VIÑAS

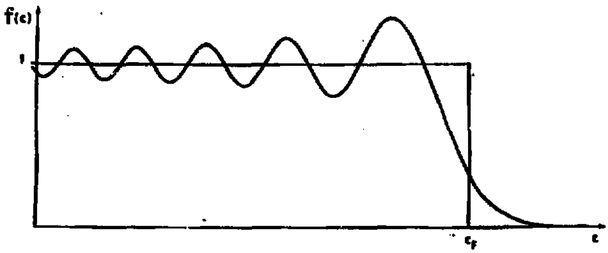
Department of theoretical physics, University of Barcelona
Diagonal 647, Barcelona 28, Spain


The Friedel oscillations are interference effects on the density of a half infinite system, close to the surface. They are also present in the Wigner transform of the density matrix $f(\vec{r},\vec{p})=f(z,p_{/\!/},p_{\perp})$ where $p_{/\!/}$ and $p_{\perp}$ are the components of the momentum $\vec{p}$ respectively parallel and perpendicular to the surface of the medium infinite in the x and y directions.

For the ramp potential and the harmonic oscillator, the Wigner distribution depends only on the classical hamiltonian : therefore, in the general case a convenient choice of variables may be some combinations of V , $p_{/\!/}$ and $p_{\perp}$ such as :

$$\varepsilon = \frac{p^2}{2m} + V(z) \quad ; \quad \Theta = \arctan \frac{V(z)}{p^2/2m} \quad ; \quad \varphi = \arctan \frac{p_{\perp}}{p_{/\!/}}$$

For fixed values $\theta_0$ and $\phi_0$ of $\theta$ and $\phi$ , the Wigner distribution $f(\varepsilon,\theta_0,\phi_0)$ for a half-infinite Fermi system will show Friedel oscillations for $\varepsilon$ close to the Fermi energy $\varepsilon_F$. The figure represents qualitatively the Wigner distribution (here for the ramp potential) for $\theta = \frac{\pi}{2}$ ( or p = 0), together with the step function corresponding to the homogeneous infinite matter : the Wigner distribution coincides with the step function when $\varepsilon \to -\infty$, it exhibits the Friedel[1] oscillations with increasing amplitudes when approaching $\varepsilon_F$ and it goes smoothly to zero around $\varepsilon_F$ when $\varepsilon \to \infty$ .




·Fig. An example of Friedel oscillations in the Wigner distribution as a function of ε (in arbitrary units) together with the unit step function, for $\vec{p} = 0$.

The $\hbar$ - expansion of the Wigner distribution :

$$f(\vec{r},\vec{p}) = \hat{\rho}_W = [\Theta(\varepsilon_F - \hat{H})]_W \qquad (1)$$

can be obtained formally from the Taylor expansion of the step function $\theta$ around the classical hamiltonian $\varepsilon = \hat{H}_W$ (the index W stands for the Wigner transforms)

$$f(\vec{r},\vec{p}) = \Theta(\varepsilon_F - \varepsilon) + (\hat{H} - \varepsilon)_W \, \delta(\varepsilon_F - \varepsilon) + \frac{1}{2!}\left[(\hat{H} - \varepsilon)^2\right]_W \delta'(\varepsilon_F - \varepsilon) + \dots$$

$$= \Theta(\varepsilon_F - \varepsilon) + \frac{\hbar^2}{4m}\Delta V \, \delta'(\varepsilon_F - \varepsilon) + \frac{\hbar^2}{24m}\left[(\vec{\nabla}V)^2 + m\left(\frac{\vec{p}}{m}\vec{\nabla}\right)^2 V\right]\delta''(\varepsilon_F - \varepsilon) + \dots \qquad (2)$$

This is a distribution representation of the density matrix which must contain the effects of the Friedel oscillations. In order to get more insight into the validity of this expansion, we want to derive it in the same way as the low temperature expansion of the Fermi function:

$$F(\varepsilon) = \left[1 + \exp\frac{\varepsilon - \varepsilon_F}{T}\right]^{-1} = \Theta(\varepsilon_F - \varepsilon) + \frac{\pi^2 T^2}{6}\,\delta'(\varepsilon_F - \varepsilon) + \dots \tag{3}$$

If we consider an arbitrary function $g(\varepsilon)$, its mean value :

$$\langle g(\varepsilon)\rangle = \int_0^\infty d\varepsilon\; g(\varepsilon)\, F(\varepsilon) \tag{4}$$

can be written exhibiting the step function :

$$\langle g(\varepsilon)\rangle = \int_0^\infty d\varepsilon\; g(\varepsilon)\Theta(\varepsilon_F - \varepsilon) + \int_0^\infty d\varepsilon\, g(\varepsilon)\,[F(\varepsilon) - \Theta(\varepsilon_F - \varepsilon)] \tag{5}$$

If the diffuseness of the Fermi function is small, the difference $(F - \theta)$ is concentrated around $\varepsilon = \varepsilon_F$, and the lower limit of the second integral can be extended from 0 to $-\infty$ with only a small error. Furthermore, if $g(\varepsilon)$ is a smooth function around $\varepsilon_F$, it can be expanded in powers of $(\varepsilon - \varepsilon_F)$ :

$$\langle g(\varepsilon)\rangle \simeq \int_0^\infty d\varepsilon\, g(\varepsilon)\Theta(\varepsilon_F - \varepsilon) + \int_{-\infty}^{+\infty} d\varepsilon\left[g(\varepsilon_F) + (\varepsilon - \varepsilon_F)g'(\varepsilon_F) + \dots\right]\left[F(\varepsilon) - \Theta(\varepsilon_F - \varepsilon)\right]$$

The difference $(F - \theta)$ being an odd function in the variable $(\varepsilon - \varepsilon_F)$, we obtain :

$$\langle g(\varepsilon)\rangle \simeq \int_0^\infty d\varepsilon\left[g(\varepsilon)\Theta(\varepsilon_F - \varepsilon) + g'(\varepsilon_F)\frac{\pi^2 T^2}{6} + \frac{g'''(\varepsilon_F)}{3!}\frac{7\pi^4 T^4}{60} + \dots\right] \tag{6}$$

Comparison between (6) and (4) leads to the expansion (3), which is valid with the following conditions :

- small diffuseness of the Fermi function, that means :

$$T/\varepsilon_F \ll 1 \tag{7}$$

- use for the calculation of the mean value of functions $g(\varepsilon)$ which are smooth around the Fermi energy, that means that just a few terms are necessary in the Taylor expansion of g, or :

$$g^{(n)}(\varepsilon_F)/[\varepsilon_F^m \, g^{(n+m)}(\varepsilon_F)] \ll 1 \qquad (m>n) \tag{8}$$

The same procedure can be applied to get the $\hbar$ - expansion of the Wigner density for the special example of the ramp - potential $V(z) = a\,z$. In this case, the Wigner density, which depends only on the classical hamiltonian is the integral Airy function and can be written as an inverse Laplace transform :

$$f(\varepsilon) = \mathcal{L}^{-1}_{\beta \to \varepsilon_F}\left[\frac{e^{-\beta\varepsilon}}{\beta}\, e^{\beta^3/3\delta^3}\right] \quad ; \quad \left(\delta^3 = \frac{8m}{\hbar^2 a^2}\right) \tag{9}$$

Proceeding as in the case of the Fermi function for the mean value of an arbitrary function $g(\varepsilon)$, one obtains :

$$\langle g(\varepsilon)\rangle = \int_{-\infty}^{+\infty} d\varepsilon \;\, g(\varepsilon)\; f(\varepsilon) \tag{10}$$

$$= \int_{-\infty}^{+\infty} d\varepsilon\, g(\varepsilon)\Theta(\varepsilon_F-\varepsilon) + \sum_{n=0}^{\infty}\frac{g^{(n)}(\varepsilon_F)}{n!}\int_{-\infty}^{+\infty} d\varepsilon(\varepsilon-\varepsilon_F)^n\left[f(\varepsilon)-\Theta(\varepsilon_F-\varepsilon)\right]$$

Using for f and $\theta$ their expression as inverse Laplace transforms gives the moments (second integral in 10) :

$$\overline{X^n} = \int_{-\infty}^{+\infty} dx\;\, x^n\, \frac{1}{2i\pi}\int_{c-i\infty}^{c+i\infty} d\beta\; \frac{e^{\beta^3/3\delta^3}-1}{\beta}\, e^{-\beta x} \tag{11}$$

Provided that the integrals converge, the order of integrations may be interchanged and, because the integrant has no pole, the $\beta$ integration may be performed along the imaginary axis ($\beta = it$). With the help of :

$$\int_{-\infty}^{+\infty} dx \; x^n \; e^{ixt} = (-i)^n \; 2\pi \, \delta^{(n)}(t) \qquad (12)$$

one gets :

$$\overline{X^n} = i^{n-1} \, (-1)^n \left\{ \frac{d^n}{dt^n} \; \frac{e^{-it^3/3s^3} - 1}{t} \right\}_{t=0} \qquad (13)$$

which leads to

$$f(\varepsilon) = \Theta(\varepsilon_F - \varepsilon) + \frac{\hbar^2 a^2}{24m} \; \delta''(\varepsilon_F - \varepsilon) + \cdots \qquad (14)$$

This is the expansion eq. 2 for the case of the linear potential.

Following the conditions for the Fermi function, this expansion (eq. 14) may be used only for rather smooth functions $g(\varepsilon)$ and if the range $\Delta$ over which f decreases to zero is small as compared to the Fermi energy : $\Delta/\varepsilon_f \ll 1$. In this case, in the calculation of the mean value of g $(\varepsilon)$, the Friedel oscillations are accounted to any desired accuracy, depending on the order to which expansion (14) is pushed.

For a general potential, with the help of the Bloch density $C^{(\beta)} = e^{-\beta \hat{H}}$

$$f(\varepsilon, \Theta, \varphi) = \mathcal{L}^{-1}_{\beta \to \varepsilon_F} \left[ \frac{C_w^{(\beta)}}{\beta} \right] \qquad (15)$$

and the moments $\overline{X^n}$ now read

$$\overline{X^n} = \int_{-\infty}^{+\infty} dx \; x^n \, \frac{1}{2i\pi} \int_{c-i\infty}^{c+i\infty} d\beta \; \frac{e^{\beta(x+\varepsilon_F)} \, C_w^{(\beta)} - 1}{\beta} \; e^{-\beta x} \qquad (16)$$

The study of the Woods-Saxon potential is now in hand and preliminary results show that all powers of $\hbar$ contribute to any derivative $\delta^{(k)}\,(\varepsilon_F - \varepsilon)$. Furthermore, similar to eq. 12, the integration over X must lead to a function of $\beta$ with a sharp maximum of narrow width around $\beta = 0$ so that an expansion in powers of $\beta$ is allowed.

In conclusion, we derived the Wigner-Kirkwood expansion in complete analogy to the low temperature expansion of the Fermi function showing that $\hbar$ and T play analogous roles in both cases. In detail however the Wigner distribution close to a surface is quite different from a Fermi function and we showed for instance that the $\hbar$-expansion can account for the surface oscillations of the distribution.

## REFERENCES

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