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Static Screening in a Degenerate Electron Plasma

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We present a self-contained derivation of the Friedel oscillations in a degenerate ideal electron plasma using a not commonly known theorem on the asymptotic behavior of the Fourier transform of a generalized function presenting some singularities.

Keywords: Degenerate electron gas; static screening; Friedel oscillations; asymptotic behavior; random phase approximation.

1. Introduction

An electron gas is a system of identical point-like charged fermions, of mass and charge those of the electron, neutralized by a uniform, inert background of opposite charge.

Some recent studies on the electron gas or *the jellium* are about two-dimensional systems[1–8] or three-dimensional ones.[2,9–14] Here, we will just consider a degenerate ideal electron gas in three dimensions.

We present a self-contained derivation of the Lindhard theory of static screening in a degenerate ideal electron plasma which explains the nature of the Friedel oscillations. We follow Sec. 4.1 of the book "Coulomb Liquids" of March and Tosi.[15] But in the end we use a not commonly known theorem on the asymptotic behavior of the Fourier transform of a generalized function presenting some singularities.

2. A Simple Derivation

Suppose we switch on an appropriately screened test charge potential δV (actually the so-called Hartree potential) in a uniform ideal Fermi gas. The Hartree potential $\delta V(r)$ created at a distance r from a static point charge of magnitude e should be evaluated self-consistently from the Poisson equation

$$\nabla^2\delta V(r) = -4\pi e^2[\delta(\mathbf{r}) + \delta n(r)], \tag{2.1}$$

where $\delta(\mathbf{r})$ ia a Dirac delta function in three dimensions and $\delta n(r)$ is the change in electronic density induced by the foreign charge. As usual, we will adopt the notation of indicating in bold the vectors so that $r = |\mathbf{r}|$ is the modulus of the three-dimensional position vector. The electron density $n(\mathbf{r})$ may be written as

$$n(\mathbf{r}) = 2\sum_{\mathbf{k}} |\psi_{\mathbf{k}}(\mathbf{r})|^2, \tag{2.2}$$

where $\psi_{\mathbf{k}}(\mathbf{r})$ denotes single-electron orbitals, the sum over $\mathbf{k}$ is restricted to occupied orbitals ($|\mathbf{k}| \leq k_F$, k_F Fermi wave vector) and the factor 2 comes from the sum over spin orientations and is needed for the paramagnetic state (equal population of up and down spins) taken under examination. We must now calculate how the orbitals in the presence of the foreign charge, differ from plane waves $\exp(i\mathbf{k}\cdot\mathbf{r})$.

We use for this purpose the Schrödinger equation

$$\nabla^2\psi_{\mathbf{k}}(\mathbf{r}) + \left[k^2 - \frac{2m}{\hbar^2}\delta V(r)\right]\psi_{\mathbf{k}}(\mathbf{r}) = 0, \quad (2.3)$$

having imposed that the orbitals reduce to plane waves with energy $\hbar^2k^2/(2m)$ at large distance.[a]

With the aforementioned boundary condition, the Schrödinger equation may be converted into an integral equation

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}}e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{2m}{\hbar^2}\int G_k(|\mathbf{r}-\mathbf{r}'|) \times \delta V(r')\psi_{\mathbf{k}}(\mathbf{r}')d\mathbf{r}', \quad (2.4)$$

where Ω is the volume of the system and we have the "spherical wave" solution $G_k(r) = -\exp(ikr)/(4\pi r)$. Here, we used the property $\nabla^2 v(r) = -4\pi\delta(\mathbf{r})$ for the Coulomb potential $v(r) = 1/r$ in three dimensions, or in Fourier q-space $q^2v(q) = 4\pi$. So that in the $k \to 0$ limit $G_k(r)$ reduces to $-v(r)/(4\pi)$. And we used the property of the Fourier transform to change a convolution into a product. After all, note that $\nabla^2 G_k(r) = -k^2G_k(r) + \delta(\mathbf{r})$, or in Fourier q-space $(k^2 - q^2)G_k(q) = 1$.

Within linear response theory, we can replace $\psi_{\mathbf{k}}(\mathbf{r})$ by $\exp(i\mathbf{k}\cdot\mathbf{r})/\sqrt{\Omega}$ inside the integral. This yields (see Appendix A)

$$\delta n(r) = -\frac{mk_F^2}{2\pi^3\hbar^2}\int j_1(2k_F|\mathbf{r}-\mathbf{r}'|)\frac{\delta V(r')}{|\mathbf{r}-\mathbf{r}'|^2}d\mathbf{r}', \quad (2.5)$$

with $j_1(x)$ being the first-order spherical Bessel function $[\sin(x) - x\cos(x)]/x^2$. Using this result in the Poisson equation, we get

$$\nabla^2\delta V(r) = -4\pi e^2\delta(\mathbf{r}) + \frac{2mk_F^2e^2}{\pi^2\hbar^2} \times \int j_1(2k_F|\mathbf{r}-\mathbf{r}'|)\frac{\delta V(r')}{|\mathbf{r}-\mathbf{r}'|^2}d\mathbf{r}', \quad (2.6)$$

which is easily soluble in Fourier transform (see Appendix B). Writing

$$\delta V(k) = \frac{4\pi e^2}{[k^2\varepsilon(k)]}$$

we find,

$$\varepsilon(k) = 1 + \frac{2mk_Fe^2}{\pi\hbar^2k^2} \times \left[1 + \frac{k_F}{k}\left(\frac{k^2}{4k_F^2} - 1\right)\ln\left|\frac{k-2k_F}{k+2k_F}\right|\right], \quad (2.7)$$

which is the static dielectric function in RPA.

For $k \to 0$ this expression gives $\varepsilon(k) \to 1 + k_{TF}^2/k^2$ with $k_{TF} = 3\omega_p^2/v_F^2$ (ω_p being the plasma frequency and v_F the Fermi velocity.) i.e. the result of the Thomas–Fermi theory. However, $\varepsilon(k)$ has a singularity at $k = \pm 2k_F$, where its derivative diverges logarithmically.[b] This singularity in $\delta V(k)$ determines, after Fourier transform, the behavior of $\delta V(r)$ at large r. $\delta V(r)$ turns out to be an oscillating function[16] rather than a monotonically decreasing function as in the Thomas–Fermi theory. Indeed,

$$\begin{aligned}\delta V(r) &= \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{4\pi e^2}{k^2\varepsilon(k)}e^{i\mathbf{k}\cdot\mathbf{r}} \\ &= \int_0^\infty k^2dk\int_0^\pi \sin\theta\, d\theta \times \int_0^{2\pi} d\varphi\,\frac{4\pi e^2}{(2\pi)^3k^2\varepsilon(k)}e^{ikr\cos\theta} \\ &= \frac{e^2}{\pi}\int_0^\infty dk\int_{-1}^1 d(\cos\theta)\,\frac{e^{ikr\cos\theta}}{\varepsilon(k)} \\ &= \frac{e^2}{i\pi r}\int_0^\infty dk\,\frac{e^{ikr}-e^{-ikr}}{k\varepsilon(k)} \\ &= \frac{e^2}{i\pi r}\int_{-\infty}^\infty dk\frac{e^{ikr}}{k\varepsilon(k)}, \end{aligned} \quad (2.8)$$

where we expressed the three-dimensional integral in $d\mathbf{k} = (dk)(k\,d\theta)(k\sin\theta\,d\varphi)$ with $k = |\mathbf{k}| \in [0,\infty]$, $\theta \in [0,\pi]$, and $\varphi \in [0, 2\pi]$ and we used the fact that $\varepsilon(k)$ is an even function. The integrand has non-analytic behavior at $k = \pm 2k_F$,

$$\left[\frac{1}{k\varepsilon(k)}\right]_{k\to\pm 2k_F} = -A(k-(\pm)2k_F)\ln|k-(\pm)2k_F| + \text{regular terms}, \quad (2.9)$$

[a]This approach (which lead to the Random Phase Approximation, RPA) is approximate insofar as the potential entering the Schrödinger equation has been taken as the Hartree potential, thus neglecting exchange and correlation between an incoming electron and the electronic screening cloud.

[b]The discontinuity in the momentum distribution across the Fermi surface introduces a singularity in elastic scattering processes with momentum transfer equal to $2k_F$.

with $A = B/(B + 4k_F^2)^2$ where $B = 2mk_Fe^2/(\pi\hbar^2) = k_{TF}^2/2$. Hence,

$$\begin{aligned}\delta V(r)|_{r\to\infty} &= -\frac{Ae^2}{i\pi r}\int_{-\infty}^{\infty} dk\, e^{ikr}[(k-2k_F)\ln|k-2k_F| - (k+2k_F)\ln|k+2k_F|] \\ &= -\frac{2Ae^2}{\pi r}\lim_{a\to 0^+}\int_0^{\infty} dk\, e^{-ak}\sin(kr)[(k-2k_F)\ln|k-2k_F| - (k+2k_F)\ln|k+2k_F|] \\ &= 2Ae^2\left\{\ln(2k_F)\frac{4k_F}{\pi r^2} + \frac{\cos(2k_Fr)}{r^3} + 2\frac{\cos(2k_Fr)\mathcal{I}m[E_1(i2k_Fr)]}{\pi r^3} + 2\frac{\sin(2k_Fr)\mathcal{R}e[E_1(i2k_Fr)]}{\pi r^3}\right\} \\ &= 2Ae^2\left\{\ln(2k_F)\frac{4k_F}{\pi r^2} + \frac{\cos(2k_Fr)}{r^3} - \frac{1}{\pi k_F r^4} + \mathrm{O}\left(\frac{1}{r^5}\right)\right\}, \end{aligned} \tag{2.10}$$

where $E_n(z)$ is the exponential integral function. This result is based on a theorem on Fourier transforms (see Theorem 19 in Ref. 17), stating that the asymptotic behavior of $\delta V(r)$ is determined by the low-k behavior as well as by the singularities of $\delta V(k)$, i.e. the points where it is not analytic. Obviously, in the present case, the asymptotic contribution from the singularities is dominant over the exponential decay of Thomas–Fermi type, due to the analytic part of the Fourier transform. The result (2.10) implies that the screened ion–ion interaction in a metal has oscillatory character and ranges over several shells of neighbors.

3. Conclusions

We presented a self-contained derivation of the Lindhard theory of static screening in a degenerate ideal electron plasma which explains the nature of the Friedel oscillations. This derivation can be used in statistical physics books for graduate students. We followed Sec. 4.1 of the book "Coulomb Liquids" of March and Tosi.[15]

Appendices

Appendix A

From Eqs. (2.2), (2.4) to Eq. (2.6)

Using periodic boundary conditions on the box of volume $\Omega = L^3$ containing the plasma we conclude that $\mathbf{k} = (2\pi/L)\mathbf{n}$ where $\mathbf{n}$ is a triplet of integers. Therefore, $(1/\Omega)\sum_{\mathbf{k}}\cdots \to \int_{|\mathbf{k}|<k_F} d\mathbf{k}/(2\pi)^3\cdots$. Now, using Eq. (2.4) into Eq. (2.2), we find

$$n(\mathbf{r}) = \frac{2}{\Omega}\sum_{\mathbf{k}}\left\{1 + \frac{2m}{\hbar^2}\int \delta V(r')2 \times \mathcal{R}e[G_k(|\mathbf{r}-\mathbf{r}'|)e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})}]d\mathbf{r}' + \cdots\right\}, \tag{A.1}$$

where we omitted terms of order $(\delta V)^2$. Therefore, we find

$$\begin{aligned}\delta n(r) &= \frac{4m}{\hbar^2\Omega}\sum_{\mathbf{k}}\int \delta V(r')2 \times \mathcal{R}e[G_k(|\mathbf{r}-\mathbf{r}'|)e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})}]\, d\mathbf{r}' \\ &= -\frac{4m}{\hbar^2}\int d\mathbf{r}'\,\frac{\delta V(r')}{4\pi|\mathbf{r}-\mathbf{r}'|}2 \times \mathcal{R}e\int_{|\mathbf{k}|<k_F}\frac{d\mathbf{k}}{(2\pi)^3}e^{ik|\mathbf{r}-\mathbf{r}'|}e^{i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})} \\ &= -\frac{mk_F^2}{2\pi^3\hbar^2}\int j_1(2k_F|\mathbf{r}-\mathbf{r}'|)\frac{\delta V(r')}{|\mathbf{r}-\mathbf{r}'|^2}\, d\mathbf{r}',\end{aligned} \tag{A.2}$$

where we used

$$\int_{|\mathbf{k}|<k_F} d\mathbf{k}\, e^{ikr}e^{i\mathbf{k}\cdot\mathbf{r}} = 2\pi i\frac{1 + 2k_F^2r^2 + e^{i2k_Fr}(-1 + i2k_Fr)}{4r^3}. \tag{A.3}$$

Appendix B

Derivation of the Static Dielectric Function

The Fourier transform of Eq. (2.6) gives

$$-k^2\delta V(k) = -4\pi e^2 + \frac{k_Fme^2}{\pi^2\hbar^2}I(\tilde{k})\delta V(k), \tag{B.1}$$

where $\delta V(k) = \int e^{i\mathbf{k}\cdot\mathbf{r}}\delta V(r)d\mathbf{r}$ and we used the property of the Fourier transform to change a convolution into a product to find

$$I(\tilde{k}) = \int \frac{j_1(x)}{x^2}e^{i\tilde{\mathbf{k}}\cdot\mathbf{x}}\, d\mathbf{x}, \tag{B.2}$$

where $\tilde{\mathbf{k}} = \mathbf{k}/2k_F$ and the integration is over the whole three-dimensional space so that $d\mathbf{x} = x^2\, dx \times \sin\theta\, d\theta\, d\varphi$. Since $\tilde{\mathbf{k}} \cdot \mathbf{x} = \tilde{k}x\cos\theta$ and $x = |\mathbf{x}| \in [0, \infty]$, $\theta \in [0, \pi]$, $\varphi \in [0, 2\pi]$, we find

$$I(\tilde{k}) = 4\pi \int_0^\infty \frac{j_1(x)}{\tilde{k}x} \sin(\tilde{k}x) dx = 2\pi \left[1 - \frac{\tilde{k}^2 - 1}{\tilde{k}} \mathrm{arctanh}(\tilde{k})\right]. \quad \text{(B.3)}$$

Recognizing that

$$\mathrm{arctanh}(\tilde{k}) = \frac{1}{2} \ln\left|\frac{\tilde{k}+1}{\tilde{k}-1}\right|, \quad \text{(B.4)}$$

one readily finds Eq. (2.7).

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Riccardo Fantoni *was born in Livorno on the 30 August 1970, lived in Pisa until 1995 where graduated "cum Laude" in the department of Physics of the University. Then moved as a graduate student to the University of Illinois at Urbana/Champaign until 2000 working as a Teaching and Research Assistant and in 1997 got a Master in Physics. Moved to Trieste and in 2004 got a Ph.D. in Physics. From 2005 to 2008 worked at the Chemical Physics department of the University "Ca' Foscari" of Venice as a postdoctoral research and teaching fellow. From 2009 to 2012 worked at the National Institute for Theoretical Physics of the University of Stellenbosch as a postdoctoral research fellow. In 2018 got a full professorship as a mathematics teacher in the secondary Italian school of second degree. In 2019 won the habilitation as an associate professor in theoretical physics of matter in the Italian university system.*

Aim of his research is to develop analytical and computational methods for condensed and soft matter starting from the fundamental many-body equations. Apart from the few analytically exactly solvable models our principal instruments, guided by the various sum-rules, are Integral Equation Theory, Density Functional Theory, Thermodynamic Perturbation Theory, Association Theory, and Monte Carlo simulations which can find exact properties of many-body systems. We are combining these approaches to create new methods and to test the accuracy of calculations on materials. Current studied materials include colloidal suspensions, ionic liquids, polymer mixtures, the electron fluid, the polaron, and boson fluids (like 4He, 4He-H2 mixtures,...). We investigate the structure and thermodynamic properties of the materials including their phase transitions like the gas-liquid-(glass)-solid first order ones and the superfluid-superconducting second order ones, the percolation threshold, the clustering, the localization, the demixing, the polydispersity, and surface properties. Lately he started working on Euclidean relativistic covariant and ultralocal quantum scalar field theories through Path integral Monte Carlo of lattice field theory subject to different kinds of quantization procedures.