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The Lindhard Theory of Screening to Study Effective Electron-Electron Interactions

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ABSTRACT

This research Paper explores the application of the Lindhard theory of screening to study effective electron-electron interactions in various systems. The Lindhard theory, developed by Danish physicist Jens Lindhard , describes the screening of a test charge by a surrounding electron gas. By applying this theory, we can gain insights into the behavior of electrons in different environments and understand how they interact with each other. The Lindhard theory of screening provides a fundamental understanding of electron-electron interactions within a many body electron gas.

This paper explores the theoretical underpinnings of the Lindhard theory, its mathematical formulation, and its implications for effective electron electron interactions in metals. By examining the response of an electron gas to perturbations, the lindhard function is derived, and its impact on screening the coulomb interaction is analyzed. Applications in understanding the electrical and thermal properties of metals, as well as complex phenomena like superconductivity and plasmon excitations, are discussed.

KEYWORDS: Screening Effect, Perturbations, Fermi-Direc Distribution function, Free Electron Model, Fermi operators, Hartree-Fock Hamiltonian, Bose systems, Ground state energy

1. INTRODUCTION

In condensed matter physics, understanding the interaction among electrons in a metal is crucial for explaining various physical properties, and magnetic behavior. Electrons in a metal interact via coulomb forces, but these interactions are modified by the presence of other electrons. The Lindhard theory, formulated by J.Lindhard in 1954. Let's explore the theoretical foundations of the Lindhard theory of screening to study effective electron electron interactions.

Electron-electron interactions play a crucial role in determining the properties of solids. The Lindhard theory of screening offers a powerful tool for understanding these interactions by describing how electrons screen each other charges. The electronic structure theory of metals, developed in the 1930's by Bloch , Bethe, Wilson and others, assumes that electron-electron interactions can be neglected, and that solid-state physics consists of computing and filling the electronic bands based on knowledge of crystal symmetry and atomic valence.

To a remarkably large extent , this works. In simple compounds, whether a system is an insulator or a metal can be determined reliably by determining the band filling in a noninteracting calculations .Bands gaps are sometimes difficult to calculate quantitatively but inclusion of simple renormalizations to electron band structure known as Hartree-Fock corrections, equivalent to calculate the average energy shift of a single electron in the presence of an average density determined by all other electrons, almost suffices to fix this problem.

There are two reasons why we now focus our attention on e^--e^- interactions, and why almost all problems of modern condensed matter physics as it relates to metallic system focus on this topic:

1. Why does the theory work so well in a simple system? This is far from clear. In a good metal the average interelectron distance is of the order of or smaller than the range of the interaction, e.g. the screening length $L_{scr} \sim (c/e^2m)^{1/2}\rho^{-1/6}$, where ρ is the density, of order 1 nm for typical parameters. One might therefore expect that interactions should strongly modify the picture of free electrons commonly used to describe metals.
2. More complicated systems exhibit dramatic deviations from the predictions of band theory. I refer now not simply to large quantitative errors in the position of 1-electron bonds, but to qualitative discrepancies in the behavior of the materials. The most interesting modern example is the class of compounds known as the transition metal oxides, including the cuprate materials which give rise to high-temperature superconductivity.

2. Methodology

Let's begin with the second-quantized form of the electronic Hamiltonian with 2-body interactions. I will focus on a translationally invariant system and do the calculation in momentum space. In this case as we have shown the Hamiltonian is

$$\hat{H} = \hat{T} + \hat{V}, \tag{1}$$

$$\hat{T} = = \sum_{\mathbf{k}\sigma} \left(\frac{\mathbf{k}^2}{2m}\right) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \tag{2}$$

$$\hat{V} = \frac{1}{2} \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q} \\ \sigma,\sigma'}} c^\dagger_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} V(\mathbf{q}) c_{\mathbf{k}'\sigma'} c_{\mathbf{k}+\mathbf{q}\sigma}. \tag{3}$$

The 2-body interaction $\hat{V}$ contains 4 Fermi operators c and is therefore not exactly soluble. The goal is to write down an effective 2-body Hamiltonian which takes into account the average effects of the interactions. We therefore replace the 4-Fermi interaction with a sum of all possible 2-body terms,

$$c^\dagger_1 c^\dagger_2 c_3 c_4 \simeq -\langle c^\dagger_1 c_3\rangle c^\dagger_2 c_4 - \langle c^\dagger_2 c_4\rangle c^\dagger_1 c_3 + \langle c^\dagger_1 c_4\rangle c^\dagger_2 c_3 + \langle c^\dagger_2 c_3\rangle c^\dagger_1 c_4, \tag{4}$$

where the + and − signs are dictated by insisting that one factor of -1 occur for each commutation of two fermion operators required to achieve the given ordering. This can be thought of as "mean field terms", in the spirit of Pierre Weiss, who replaced the magnetic interaction term $S_i \cdot S_j$ in a ferromagnet by $\langle S_i \rangle S_j = \langle S \rangle S_j \equiv -H_{eff} S_j$, i.e. he replaced the field S_i by its homogeneous mean value S, and was left with a term equivalent to a 1-body term corresponding to a spin in an external field which was soluble. The mean field $\langle S \rangle$ in the Weiss theory is the instantaneous average magnetization of all the other spins except the spin S_j, and here we attempt the same thing, albeit somewhat more formally.

$$\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma'}\rangle = \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle \delta_{\mathbf{kk}'}\delta_{\sigma\sigma'} \equiv n_{\mathbf{k}\sigma}\delta_{\mathbf{kk}'}\delta_{\sigma\sigma'} \qquad (5)$$

The "mean field" is the average number of particles $n_{\mathbf{k}\boldsymbol{\sigma}}$ in the state **k**σ, which will be weighted with the 2-body interaction V(**q**) to give the average interaction due to all other particle. With these arguments in mind, we use the approximate form (4) and replace the interaction $\hat{V}$ in (3) by

$$\begin{aligned}
\hat{V}_{HF} &= \frac{1}{2}\sum_{\substack{\mathbf{kk}'\mathbf{q}\\ \sigma\sigma'}} V(\mathbf{q})\Big[-\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma'}\rangle c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}+\mathbf{q}\sigma} - \langle c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}+\mathbf{q}\sigma}\rangle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma'} + \\
&\qquad + \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma}\rangle c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} + \langle c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'}\rangle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma}\Big] \\
&= -\sum_{\substack{\mathbf{kq}\\ \sigma}} V(\mathbf{q})\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma} + V(0)\sum_{\substack{\mathbf{kk}'\\ \sigma\sigma'}} \langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\rangle c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'} \\
&= \sum_{\mathbf{k}\sigma}\Big(-\sum_{\mathbf{q}} n_{\mathbf{k}-\mathbf{q}\sigma} V(\mathbf{q}) + nV(0)\Big) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \qquad (6)
\end{aligned}$$

where the total density n is defined to be $n = \Sigma_{\mathbf{k}\boldsymbol{\sigma}}\, n_{\mathbf{k}\boldsymbol{\sigma}}$. Since this is now a 1-body term of the form $\Sigma_{\mathbf{k}\boldsymbol{\sigma}}\Sigma_{HF}(\mathbf{k})a^\dagger_{\mathbf{k}\boldsymbol{\sigma}}a_{\mathbf{k}\boldsymbol{\sigma}}$, it is clear the full Hartree-Fock Hamiltonian may be written in terms of a k-dependent energy shift:

$$\begin{aligned}
\hat{H}_{HF} &= \sum_{\mathbf{k}\sigma}\left(\frac{\hbar^2 k^2}{2m} + \Sigma_{HF}(\mathbf{k})\right) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, && (7)\\
\Sigma_{HF}(\mathbf{k}) &= \underbrace{-\sum_{\mathbf{q}} n_{\mathbf{k}-\mathbf{q}\sigma} V(\mathbf{q})}_{Fock} + \underbrace{nV(0)}_{Hartree} && (8)\\
& && (9)
\end{aligned}$$

Note the Hartree or direct *Coulomb* term, which represents the average interaction energy of the electron ***kσ*** with all the other electrons in the system, is merely a constant, and as such it can be absorbed into a chemical potential. In fact it is seen to be divergent if $\boldsymbol{V(q)}$ represents the Coulomb interaction $\boldsymbol{4\pi e^2/q^2}$, but this divergence must cancel exactly with the constant arising from the sum of the self-energy of the positive background and the interaction energy of the electron gas with that background. The Fock, or exchange term is a momentum-dependent shift.

2.1 Validity of Hartree-Fock theory

Crucial question: when is such an approximation a good one for an interacting system?

The answer, curiously, turns out to be different for bosons and fermions. The HF approximation is a good one for interacting *low density Bose systems or high density Fermi systems!* Intuitively it seems obvious that if the particles are further apart on the average, they will interact less strongly and less often, so a mean field theory like Hartree-Fock theory should work well. This is true in the Bose case: the only characteristic energies are the temperature T and the zero-point energy. The latter is just the energy scale obtained by confining the particle to a cage of size the interparticle spacing r_s, i.e. $\boldsymbol{\hbar^2/(2mr_s^2)}$. The interaction is typically characterized by a *strength V* and a *range a*, and if $\mathbf{r_s} \gg \mathbf{a}$, the particles don't feel the potential much and the ground state energy, for example, of such a gas can be expanded at T = 0 in powers of a/r_s. The result is

$$E_0 = E_0^{HF} + E_{corr} \qquad (10)$$

with E_0^{HF} the ground state energy calculated in the independent particle approximation with the Hartree-Fock energy shifts, and E_{corr} the correlation energy, which is found to vary as

$$\frac{E_{corr}}{E_0^{HF}} \simeq \frac{1}{r_s^{\alpha}}, \ (\text{bosons}) \qquad (11)$$

with α = xxx, and therefore → 0 in the low density limit.

In the case of Fermions, a new energy scale arises due to the Pauli principle, namely ε_F . As the density increases, so does ε_F , which represents the average kinetic energy of electrons; this increase is faster than the increase of the correlation energy. For the electron gas with Coulomb interactions, for example, we have, in terms of the Bohr radius a_0 we have (per particle)

$$K.E. \ = \tfrac{3}{5}\varepsilon_F = \frac{2.21}{r_s^2}\,\text{Ryd} \qquad (12)$$

$$P.E.|_{HF} \quad = \quad \frac{-0.916}{r_s}\,\text{Ryd} \qquad (13)$$

and the correlation energy is given by

$$\frac{E_{corr}}{\text{Ryd}} = 0.0622 \log r_s - 0.096 + \ldots \qquad (14)$$

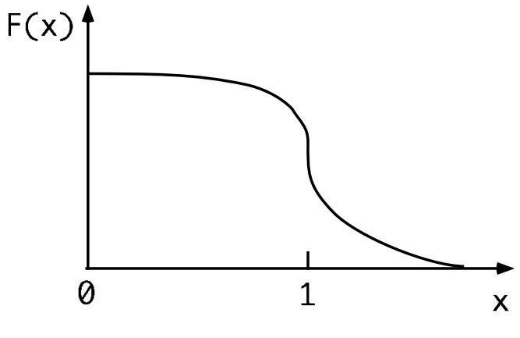
so it is clear the correlation term is less singular than the HF term in the limit $r_s \to 0$. At higher densities, particles are effectively independent.

2.2 Problem with Hartree-Fock theory

Although we argued that the Hartree-Fock approximation becomes a better approximation in the limit of low (high) density for bosons (fermions), it never becomes exact, as one can see by examining the Fourier transform of the Hartree-Fock energy shift in the presence of the bare Coulomb interaction $V(q)=4\pi e^2/q^2$. The Hartree term itself (being **k** independent) is absorbed into a redefinition of the chemical potential, so the shift is (T=0):

$$\delta\varepsilon_{\mathbf{k}} \ = \ \pm\frac{1}{L^3}\sum_{|\mathbf{k}'|<k_F}\frac{4\pi e^2}{|\mathbf{k}-\mathbf{k}'|^2} \qquad (15)$$

$$\ = \ \frac{2e^2 k_F}{\pi}F(k/k_F), \qquad (16)$$



where **F(x)** is a function which has a log divergence in slope at x = 1, i.e. at the Fermi level. This means while the energy shift might be small compared to the Fermi energy **v**ε_F , the *velocity* of an electron is

, which contains a term which is infinite $\partial\varepsilon_{\mathbf{k}}/\partial\mathbf{k}|_{k_F}$

This problem can be traced back to the long-range nature of the Coulomb force. Two electrons at large distances $\mathbf{r} - \mathbf{r'}$ don’t really feel the full $\mathbf{1/|r - r'|^2}$ but a “screened” version due to the presence of the intervening medium, i.e. The electron gas rearranges itself to cancel out the long-range part of V.

2.3 RANDOM PHASE APPROXIMATION:

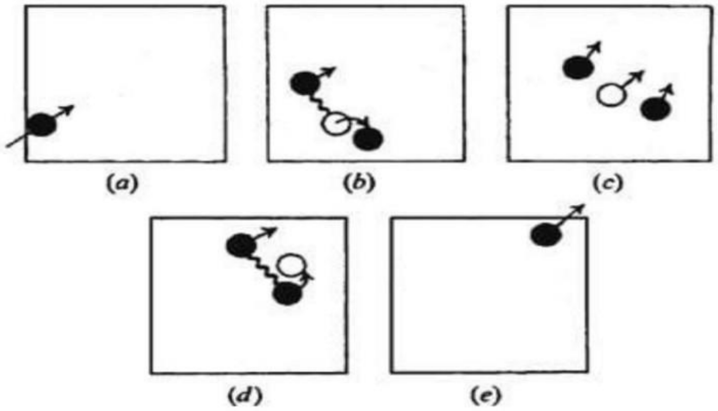
Random Phase Approximation (RPA) is an approximation for microscopic quantum mechanical interactions between electrons in matter.

Random phase approximation (RPA) is an important and widely used approximation in condensed matter physics, especially when calculating the linear response of electrons. It accounts for the microscopic quantum mechanical interactions between electrons using weak screened Coulomb interaction. It was first introduced by David Bohm and David Pines as an important result in a series of seminal papers of 1952 and 1953.

In the RPA, electrons are assumed to respond only to the total electric potential V(r) which is the sum of the external perturbing potential Vext(r) and a screening potential Vsc(r). The external perturbing potential is assumed to oscillate at a single frequency $\boldsymbol{\omega}$, so a self-consistent field (SCF) approach is possible giving a dynamic dielectric function denoted by ϵRPA (k,ω).

The assumption in RPA is that the contribution to the dielectric function from the total electric potential is assumed to average out so that only the potential at wave vector **k** contributes. This is what is meant by the random phase approximation. The resulting dielectric function correctly predicts a number of properties of the electron gas, including plasmons (see Mahan's Many-Particle Physics).

2.4 RPA AS A DIAGRAMMATIC SUMMATION:

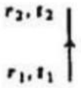


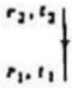
(Figure Movie of second-order propagation process in many-body system)

1. At time f_1 extra particles enters system.
2. At time t_1, extra particles interact (ways line) with a particle in the system, lifting it out of its place, thus creating a hole in the system.
3. The extra particles plus the hole and the lifted-out particle (particle-hole pair) travel through the system.
4. At time t the extra particle interacts with the lifted-out particle, knocking it back into the hole, thus destroying the particle-hole pair.
5. At time t_2, the extra particle moves out of the system.

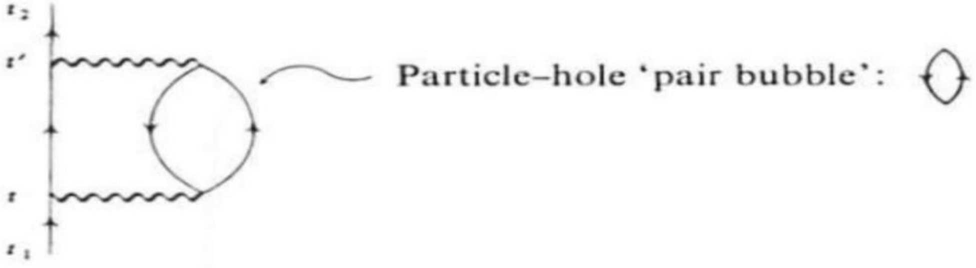
The single particle propagator for a system of many interacting particles can be dissected as a series of virtual events. (a) depicts a free propagation without interaction. The event in (b) depicts a 'second-order' propagation process (a process with two interactions).

A sequence of events means we need a time axis. Due to time reversal symmetry, electrons move forward, and holes move backward. By convention, "up" is the forward time.





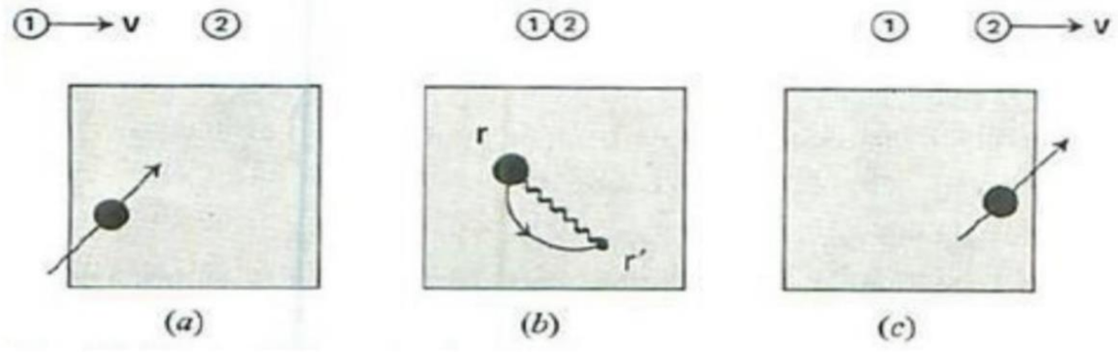
The probability amplitude attached for the above sequence of events can be represented by the diagram:



Self energy

This diagram is called the **self-energy** part because it shows the particle interacting with itself via the particle-hole pair it created in the many-body medium.

The process that involve only the one interaction is called the first order processes



(Movie of First-order process (Lower Drawing) and it's Analogy (Lipper Drawing)

(a) Extra particles enter at time t_1.
(b) At time t, the particle is at point r. It interacts with a particle at r' and charges in place with it.
(c) Extra particle leaves at time t_2.

2.5 FORMULA:

The Lindhard formula for the longitudinal dielectric function is given by

$$\epsilon(\mathbf{q},\omega) = 1 - V_{\mathbf{q}} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}}}{\hbar(\omega + i\delta) + E_{\mathbf{k}-\mathbf{q}} - E_{\mathbf{k}}}.$$

Here, ***δ*** is a positive infinitesimal constant, Vq is $V_{eff}(q)$-$V_{ind}(q)$ and f_k is the carrier distribution function which is the Fermi-Dirac distribution function for electrons in thermodynamic equilibrium. However this Lindhard formula is valid also for nonequilibrium distribution functions. It can be obtained by first-order perturbation theory and the random phase approximation (RPA).

3. RESULT AND CONCLUSION-

The Lindhard formula for the longitudinal dielectric function is given by

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Limiting cases

To understand the Lindhard formula, consider some limiting cases in 2 and 3 dimensions. The 1- dimensional case is also considered in other ways.

Long wavelength limit

In the long wavelength limit (q → 0), Lindhard function reduces to

$$\epsilon(\mathbf{q} = 0, \omega) \approx 1 - \frac{\omega_{\mathrm{pl}}^2}{\omega^2},$$

where is this the three-dimensional plasma frequency (in SI units, replace

$$\omega_{\mathrm{pl}}^2 = \frac{4\pi e^2 N}{L^3 m}$$

the factor 4 by 1/For two-dimensional systems,

$$\omega_{\mathrm{pl}}^2(\mathbf{q}) = \frac{2\pi e^2 n q}{\epsilon m}.$$

This result recovers the plasma oscillations from the classical dielectric function from Drude model and from the quantum mechanical free electron model.

Static Limit

Consider the static limit (ω + *i*δ → 0)

The Lindhard formula becomes

$$\epsilon(\mathbf{q}, \omega = 0) = 1 - V_{\mathbf{q}} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}}}{E_{\mathbf{k}-\mathbf{q}} - E_{\mathbf{k}}}.$$

Inserting the above equalities for the denominator and numerator, we obtain

$$\epsilon(\mathbf{q},0) = 1 - V_{\mathbf{q}} \sum_{\mathbf{k},i} \frac{-q_i \frac{\partial f}{\partial k_i}}{-\frac{\hbar^2 \mathbf{k}\cdot\mathbf{q}}{m}} = 1 - V_{\mathbf{q}} \sum_{\mathbf{k},i} \frac{q_i \frac{\partial f}{\partial k_i}}{\frac{\hbar^2 \mathbf{k}\cdot\mathbf{q}}{m}}$$

Assuming a thermal equilibrium Fermi–Dirac carrier distribution, we get

$$\sum_i q_i \frac{\partial f_{\mathbf{k}}}{\partial k_i} = -\sum_i q_i \frac{\partial f_{\mathbf{k}}}{\partial \mu} \frac{\partial E_{\mathbf{k}}}{\partial k_i} = -\sum_i q_i k_i \frac{\hbar^2}{m} \frac{\partial f_{\mathbf{k}}}{\partial \mu}$$

here, we used $E_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}$ and $\frac{\partial E_{\mathbf{k}}}{\partial k_i} = \frac{\hbar^2 k_i}{m}$.

Therefore,

$$\epsilon(\mathbf{q},0) = 1 + V_{\mathbf{q}} \sum_{\mathbf{k},i} \frac{q_i k_i \frac{\hbar^2}{m} \frac{\partial f_{\mathbf{k}}}{\partial \mu}}{\frac{\hbar^2 \mathbf{k}\cdot\mathbf{q}}{m}} = 1 + V_{\mathbf{q}} \sum_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}}{\partial \mu} = 1 + \frac{4\pi e^2}{\epsilon q^2} \frac{\partial}{\partial \mu} \frac{1}{L^3} \sum_{\mathbf{k}} f_{\mathbf{k}}$$
$$= 1 + \frac{4\pi e^2}{\epsilon q^2} \frac{\partial}{\partial \mu} \frac{N}{L^3} = 1 + \frac{4\pi e^2}{\epsilon q^2} \frac{\partial n}{\partial \mu} \equiv 1 + \frac{\kappa^2}{q^2}.$$

Here, **κ** is the 3D screening wave number (3D inverse screening length) defined as

$$\kappa = \sqrt{\frac{4\pi e^2}{\epsilon} \frac{\partial n}{\partial \mu}}.$$

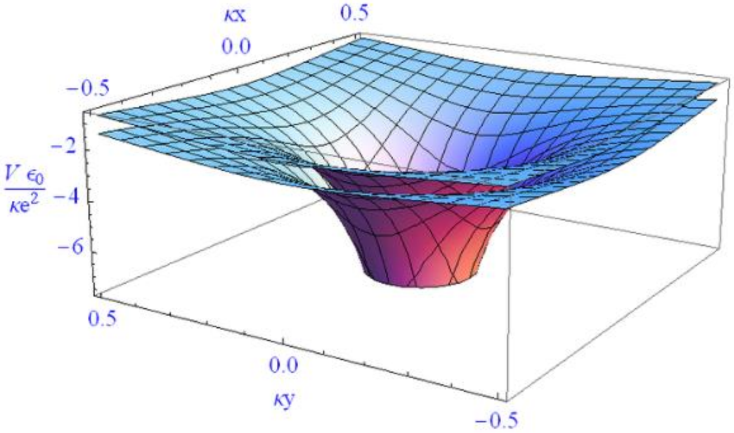
Then, the 3D statically screened Coulomb potential is given by

$$V_s(\mathbf{q}, \omega = 0) \equiv \frac{V_{\mathbf{q}}}{\epsilon(\mathbf{q},0)} = \frac{\frac{4\pi e^2}{\epsilon q^2 L^3}}{\frac{q^2 + \kappa^2}{q^2}} = \frac{4\pi e^2}{\epsilon L^3} \frac{1}{q^2 + \kappa^2}.$$

And the inverse Fourier transformation of this result gives

$$V_s(r) = \sum_{\mathbf{q}} \frac{4\pi e^2}{L^3 (q^2 + \kappa^2)} e^{i\mathbf{q}\cdot\mathbf{r}} = \frac{e^2}{r} e^{-\kappa r}$$

known as the Yukawa potential. Note that in this Fourier transformation, which is basically a sum over all **q**, we used the expression for small |**q**| for every value of **q** which is not correct.



Statically screened potential(upper curved surface) and Coulomb potential(lower curved surface) in three dimensions

For a degenerate Fermi gas (T=0), the Fermi energy is given by

$$E_{\mathrm{F}} = \frac{\hbar^2}{2m}(3\pi^2 n)^{\frac{2}{3}},$$

So the density is,

$$n = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}E_{\mathrm{F}}\right)^{\frac{3}{2}}.$$

$$\text{At } T\text{=0, } E_{\mathrm{F}} \equiv \mu \text{, so } \frac{\partial n}{\partial \mu} = \frac{3}{2}\frac{n}{E_{\mathrm{F}}}$$

Inserting this into the above 3D screening wave number equation, we obtain

$$\boxed{\kappa = \sqrt{\frac{4\pi e^2}{\epsilon}\frac{\partial n}{\partial \mu}} = \sqrt{\frac{6\pi e^2 n}{\epsilon E_{\mathrm{F}}}}.}$$

This result recovers the 3D wave number from Thomas–Fermi screening.

For reference, Debye–Hückel screening describes the non-degenerate limit case. The result

$$; \kappa = \sqrt{\frac{4\pi e^2 n\beta}{\epsilon}}$$

is known as the 3D Debye–Hückel screening wave number.8

In two dimensions, the screening wave number is

$$\kappa = \frac{2\pi e^2}{\epsilon}\frac{\partial n}{\partial \mu} = \frac{2\pi e^2}{\epsilon}\frac{m}{\hbar^2 \pi}(1 - e^{-\hbar^2 \beta \pi n/m}) = \frac{2me^2}{\hbar^2 \epsilon} f_{k=0}.$$

Note that this result is independent of n.

The lindhard theory of screening is a cornerstone in the study of effective electron-electron interactions in a many body electron system by deriving the Lindhard function and analyzing its impact on the dielectric function and screened coulomb potential and the power of the lindhard theory of screening in studying effective electron-electron interactions in solid.

The Lindhard screening theory is used to describe the collective electronic response of a many electron system to an external perturbation, such as an electric field. In conclusion, this theory provides a framework for understanding how the electrons in a material screen or shield each other from external influences.

It is so useful in the study of plasmas,semiconductors and metals,where electron-electron interactions are important. Lindhard screening theory has been a valuable tool in condensed matter physics and solid state physics, helping to explain phenomena like the dielectric response of materials and electron-electron interactions.

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