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DISCRETE APPROACH TO INCOHERENT EXCITATIONS IN CONDUCTORS

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Dedicated to Professor Kseno Ilakovac on the occasion of his 70$^{\rm th}$ birthday

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While keeping the discreteness of the reciprocal space, we calculate the spectrum of incoherent electron-hole excitations in the conducting Fermi liquids. The method is illustrated on the well-known jellium model within the random phase approximation. It also leads to the formulation of a sum rule from which we get the details of the dispersion curve for the collective plasmon mode. The notion of time averaging in the discrete approach is briefly recalled.

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1. Introduction

The electron-hole excitations in conductors invoke in the frequency dependence of dielectric function $\epsilon(\boldsymbol{k}, \omega)$ a dense alternation of poles and zeros at the scale of discreteness of the reciprocal space [1]. Usually this complex mathematical problem is avoided by making the standard procedure of continuation of the wave vector variable $\boldsymbol{k}$ which is well founded for macroscopic systems, and in addition includes the standard proposition allowing for the irreversibility in the thermodynamic limit [2]. By this, the dense set of poles and zeros is eliminated, and $\epsilon(\boldsymbol{k}, \omega)$ becomes an analytic function. In particular, within the random phase approximation (RPA) for jellium, which will be followed here, Im ϵ is a continuous function of $\boldsymbol{k}$ and ω in the range of variables covering the so-called electron-hole continuum.

Although cumbersome at first sight, the discrete presentation of dielectric response still appears to be advantageous and physically more transparent in some treatments, like in the calculations of the cohesive energy [3, 4] and one-particle spectral function [5] in the single-band and multi-band systems. In the present work we show how the method developed in Refs. [4, 5] reproduces some well-known results for the jellium model. In particular, we derive an explicit expression for energies of incoherent excitations, which is, of course, not attainable after continuation. This leads to the formulation of a sum rule which enables a direct determination of the dispersion curve for the collective excitation (i. e. plasmon in the present example). The particular detail which then can be followed in a transparent way is the cross-over of the plasmon dispersion from the collective to the incoherent regime as the wave vector increases, the subject which was often exposed incorrectly or imprecisely in literature.

In Sect. 2 we start with the formulation of the problem and continue with the explicit calculation of energies of incoherent excitations. Section 3 contains the formulation of the sum rule, the analysis of the plasmon dispersion and the short note on the calculation of Im ϵ in the discrete approach. Concluding remarks are given in Sect. 4.

2. *Incoherent excitations*

We start from the well-known RPA dielectric function for the jellium [1]. The excitation energy for a given value of the wave vector $\boldsymbol{q}$ is the solution of the equation $\varepsilon(\boldsymbol{q},\omega)=0$ in the frequency variable ω. Let us write this equation in the form

$$\varepsilon(\boldsymbol{q},\omega) = 1 - \frac{4e^2}{\pi q^2 L}\sum_{k_\parallel=-k_F}^{k_F} g(k_\parallel,\boldsymbol{q})\frac{E(k_\parallel,\boldsymbol{q})}{[\omega+\mathrm{i}\ \mathrm{sign}(\omega)\eta]^2 - E^2(k_\parallel,\boldsymbol{q})} = 0\,, \tag{1}$$

where L^3 is the volume of the system. We keep throughout this text the discrete summation in terms of the wave vector component parallel to $\boldsymbol{q}$,

$$k_\parallel = n\frac{2\pi}{L}\ \ ,\ \ n\in Z. \tag{2}$$

The equation $k_\parallel = constant$ defines the locus of the constant electron-hole excitation energy

$$E(k_\parallel,\boldsymbol{q}) = \frac{1}{2m}(2k_\parallel+q)q\,, \tag{3}$$

i.e., the summation in Eq. (1) goes over all such loci. As shown in Fig. 1, the locus for given values of q and $k_\parallel$ is either circular [for $E(k_\parallel,\boldsymbol{q}) > (k_F^2-k_\parallel^2)/2m$] or annular [for $E(k_\parallel,\boldsymbol{q}) < (k_F^2-k_\parallel^2)/2m$] surface, centered at $k_\parallel$. The radius of the former is $k_{\perp M} \equiv \sqrt{k_F^2 - k_\|^2}$, while the latter is bounded by concentric circles with radii $k_{\perp M}$ and $k_{\perp m} \equiv \sqrt{k_F^2 - (k_\| + q)^2}$.

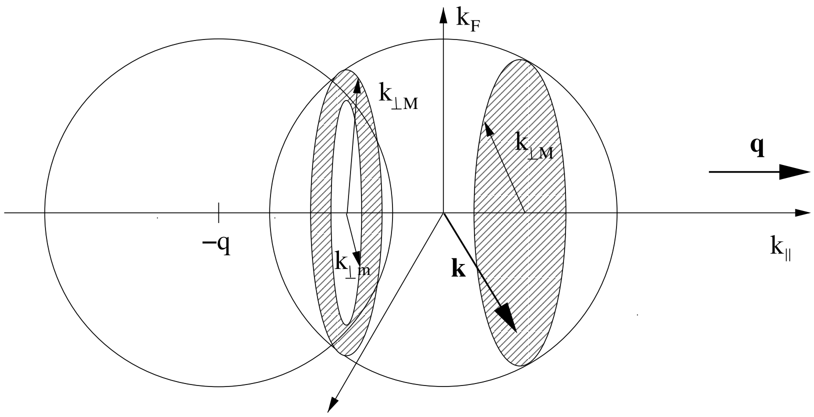

Fig. 1. The loci of the constant electron-hole excitation energies, containing all wave vectors $\boldsymbol{k}$ *with a same energy* $E(\boldsymbol{k},\boldsymbol{q}) = E(\boldsymbol{k}+\boldsymbol{q}) - E(\boldsymbol{k}) = (2k_\| + q)q/2m = const.$

The number of the points multiplied with the elementary surface $(2\pi/L)^2$ of the reciprocal space in a given locus is

$$g(k_\|, \boldsymbol{q}) = \begin{cases} (k_F^2 - k_\|^2)\pi & k_F > k_\| > k_F - q \\ (2k_\| + q)q\pi & k_F - q > k_\| > -q/2 \end{cases} \quad \text{for } \; q < 2k_F\,, \tag{4}$$

and $$g(k_\|, \boldsymbol{q}) = (k_F^2 - k_\|^2)\pi \quad \text{for } \; q > 2k_F\,. \tag{5}$$

The dielectric function (1) diverges at energies which are infinitesimally close to the values of electron-hole excitation energies (3) at the real ω-axis. The energy difference between neighboring poles (3) is

$$\Delta E(\boldsymbol{q}) = E(k_\| + 2\pi/L, \boldsymbol{q}) - E(k_\|, \boldsymbol{q}) = \frac{2\pi q}{mL}. \tag{6}$$

Between each such pair of neighboring poles (3), there should be a zero of the dielectric function. In other words, all solutions of the equation $\varepsilon(\boldsymbol{q},\omega) = 0$, except the largest one, lie between neighboring electron-hole energies. Let us denote these zeros by $\Omega(k_\|, \boldsymbol{q})$, and write

$$\Omega(k_\|, \boldsymbol{q}) + \mathrm{i}\ \mathrm{sign}(\Omega)\eta = E(k_\|, \boldsymbol{q}) + \Theta(k_\|, \boldsymbol{q})\Delta E(k_\|, \boldsymbol{q})\,, \tag{7}$$

with $0 < \Theta(k_\|, \boldsymbol{q}) < 1$. Let us remind that, in contrast to these *incoherent excitations*, the excitation with the largest energy can be macroscopically (with respect to $1/L$) far from its closest electron-hole counterpart, $E(k_F, \boldsymbol{q})$. Such isolated zero is a *collective excitation*, i. e. plasmon in the present jellium model.

An approximate expression for the energies of incoherent excitations follows after retaining the ω-dependence only in those terms of Eq. (1) which contain nearest neighboring poles to a given zero $\Omega(k_\parallel, \boldsymbol{q})$, i. e. only in terms with $E(k_\parallel, \boldsymbol{q})$ and $E(k_\parallel + 2\pi/L, \boldsymbol{q})$. In terms with wave vectors different from $k_\parallel$ or $k_\parallel + 2\pi/L$, we substitute $\omega + \mathrm{i}\ \mathrm{sign}(\omega)\eta$ with $E(k_\parallel, \boldsymbol{q})$. The validity of this approximative step is discussed in the Appendix. Eq. (1) now reduces to

$$1 - \frac{4}{\pi^2 q^2 a_0}\left\{F(k_\parallel, \boldsymbol{q}) + \frac{\pi}{mL}\left[\frac{g(k_\parallel, \boldsymbol{q})E(k_\parallel, \boldsymbol{q})}{[\omega + \mathrm{i}\ \mathrm{sign}(\omega)\eta]^2 - E^2(k_\parallel, \boldsymbol{q})} + \frac{g(k_\parallel + \frac{2\pi}{L}, \boldsymbol{q})E(k_\parallel + \frac{2\pi}{L}, \boldsymbol{q})}{[\omega + \mathrm{i}\ \mathrm{sign}(\omega)\eta]^2 - E^2(k_\parallel + \frac{2\pi}{L}, \boldsymbol{q})}\right]\right\} = 0, \tag{8}$$

where $a_0 = 1/me^2$ is the Bohr radius and

$$F(k_\parallel, \boldsymbol{q}) = \frac{\pi}{mL}\left[\sum_{k'_\parallel = -k_F}^{k_\parallel - 2\pi/L} \frac{g(k'_\parallel, \boldsymbol{q})E(k'_\parallel, \boldsymbol{q})}{E^2(k_\parallel, \boldsymbol{q}) - E^2(k'_\parallel, \boldsymbol{q})} + \sum_{k'_\parallel = k_\parallel + 4\pi/L}^{k_F} \frac{g(k'_\parallel, \boldsymbol{q})E(k'_\parallel, \boldsymbol{q})}{E^2(k_\parallel, \boldsymbol{q}) - E^2(k'_\parallel, \boldsymbol{q})}\right]. \tag{9}$$

With the most divergent terms singled out, we can now make a continuation of the residual sums in Eq. (9) by replacing each term with the integral over the interval $2\pi/L$. Choosing to replace a term characterized by the discrete value $k'_\parallel$ with the integral from $k'_\parallel - 2\pi/L$ to $k'_\parallel$, we come to the expression

$$F(k_\parallel, \boldsymbol{q}) = \frac{1}{2m}\left[\int_{-k_F}^{k_\parallel - 2\pi/L} \mathrm{d}\, k'_\parallel\ \frac{g(k'_\parallel, \boldsymbol{q})E(k'_\parallel, \boldsymbol{q})}{E^2(k_\parallel, \boldsymbol{q}) - E^2(k'_\parallel, \boldsymbol{q})} + \int_{k_\parallel + 2\pi/L}^{k_F} \mathrm{d}\, k'_\parallel\ \frac{g(k'_\parallel, \boldsymbol{q})E(k'_\parallel, \boldsymbol{q})}{E^2(k_\parallel, \boldsymbol{q}) - E^2(k'_\parallel, \boldsymbol{q})}\right], \tag{10}$$

where $k_\parallel - 2\pi/L$ and $k_\parallel + 2\pi/L$ are the lower and upper boundaries of the interval that corresponds to the missing terms $k_\parallel$ and $k_\parallel + 2\pi/L$ in the sum (9). We note that the final result of integration in Eq. (10) does not depend on the choice of integration boundaries for $2\pi/L$ intervals, as specified above.

Since the primitive function in the above integral is odd with respect to the pole at $k'_\parallel$, the expression (10) can be rewritten in the form

$$F(k_\parallel, \boldsymbol{q}) = \frac{1}{2m}\int_{-k_F}^{k_F} \mathrm{d}\, k'_\parallel\ \frac{g(k'_\parallel, \boldsymbol{q})E(k'_\parallel, \boldsymbol{q})}{E^2(k_\parallel, \boldsymbol{q}) - E^2(k'_\parallel, \boldsymbol{q})}\,. \tag{11}$$

After elementary integration, we get

$$F(k_\parallel,\boldsymbol{q}) = \frac{\pi}{4}\left[-2k_F - \frac{k_F^2-k_\parallel^2}{q}\ln\left|\frac{(k_F-k_\parallel)(k_F+k_\parallel+q)}{(k_F+k_\parallel)(k_F-k_\parallel-q)}\right| \right. \\ \left. +(2k_\parallel+q)\ln\left|\frac{k_F+k_\parallel+q}{k_F-k_\parallel-q}\right|\right]. \tag{12}$$

Furthermore, by solving the biquadratic Eq. (8), we get for the function $\Theta(k_\parallel,\boldsymbol{q})$ in Eq. (7) the expression

$$\Theta(k_\parallel,\boldsymbol{q}) = \frac{1}{2}[1+x-\mathrm{sign}(x)\sqrt{1+x^2}], \tag{13}$$

where

$$x \equiv \frac{2\pi g(k_\parallel,\boldsymbol{q})}{q[\pi^2q^2a_0-4F(k_\parallel,\boldsymbol{q})]}\,. \tag{14}$$

Evidently, Θ varies in the range $(0,1)$ in accordance with the starting assumption. More precisely,

$$\begin{array}{lcll} 0<\Theta(k_\parallel,\boldsymbol{q})<1/2 & & & >0 \\ \Theta(k_\parallel,\boldsymbol{q})=1 & \text{for} & \pi^2q^2a_0-4F(k_\parallel,\boldsymbol{q}) & =0\ . \\ 1/2<\Theta(k_\parallel,\boldsymbol{q})<1 & & & <0 \end{array} \tag{15}$$

The above results can be written in a more explicit way in the limits $q << k_F$ and $q >> 2k_F$. In the former case and for $k_\parallel \ll k_F$, the expression (12) reduces to

$$F(k_\parallel,\boldsymbol{q}) \approx -\pi k_F + \frac{\pi k_\parallel^2}{2k_F} + \frac{\pi(2k_\parallel+q)(k_\parallel+q)}{2k_F}\,, \tag{16}$$

and the leading term in the energy of incoherent excitations is

$$\Omega(k_\parallel,\boldsymbol{q}) = E(k_\parallel,\boldsymbol{q}) + \frac{\pi q(2k_\parallel+q)}{2k_FmL}\,, \tag{17}$$

i.e., the zeros of $\epsilon(\omega,\boldsymbol{k})$ in the ω-plane lie very close to the corresponding electron-hole excitation poles. Here and further on, we omit for simplicity the infinitesimal imaginary part in excitation energies (7).

As the wave number $k_\parallel$ increases, the energy of incoherent excitations moves gradually towards the first higher neighboring electron-hole excitation. For $k_\parallel$ close to k_F and for $k_F \gg q \gg k_F-k_\parallel$, the function (12) reduces to

$$F(k_\parallel,\boldsymbol{q}) \approx \frac{\pi(2k_F+q)}{4}\ln\frac{2k_F+q}{q} - \frac{\pi k_F}{2} - \frac{\pi k_F(k_F-k_\parallel)}{2q}\ln\frac{k_F-k_\parallel}{q}\,. \tag{18}$$

Keeping only the leading term in the above expression, the approximate expression for the corresponding energies of incoherent excitation reads

$$\Omega(k_\parallel,\boldsymbol{q}) = E(k_\parallel+2\pi/L,\boldsymbol{q}) - \frac{2\pi(k_F-k_\parallel)}{mL\ln(2k_F/q)}\,, \tag{19}$$

i.e., these energies are very close to the energies of the first larger neighboring electron-hole excitations.

In the latter case, $q >> 2k_F$, Eq. (12) reduces to

$$4F(k_\parallel, \boldsymbol{q}) \approx \pi \left(\frac{2k_\parallel k_F}{q} - \frac{k_F^2 - k_\parallel^2}{q} \ln \frac{k_F - k_\parallel}{k_F + k_\parallel} \right) \ll \pi^2 q^2 a_0. \tag{20}$$

Energies of incoherent excitations are then given by

$$\Omega^2(k_\parallel, \boldsymbol{q}) - E^2(k_\parallel, \boldsymbol{q}) = \frac{4e^2}{\pi L q^2} g(k_\parallel, \boldsymbol{q}) \left[1 + \frac{4me^2 F(k_\parallel, \boldsymbol{q})}{\pi^2 q^2} \right] E(k_\parallel, \boldsymbol{q}), \tag{21}$$

i.e., they are very close to their electron-hole counterparts for all values of $k_\parallel$. The physical reason for this small departure of incoherent excitations from bare electron-hole ones is the weakness of the bare Coulomb interaction $4\pi e^2/q^2$ in this regime.

It follows from the foregoing analysis that the regime of small values of q qualitatively differs from that of large ones. In the former case, the energy of incoherent excitations moves from their electron-hole counterpart towards the first larger neighboring electron-hole excitation, crossing the half-width $\Delta E(\boldsymbol{q})/2$ (Eq. 6), as $k_\parallel$ moves from the lower bound, $-q$, to the upper bound, $k_F - 2\pi/L$. On the contrary, in the latter case, it does not cross the half-width. It is interesting to estimate the value of the wave vector $q_{\rm cr}$ which roughly separates these two regimes. To this end, we note that in the regime of small values of q the difference between the energy of incoherent excitation and its electron-hole counterpart has the largest value for $k_\parallel \approx k_F$. Let us define the critical wave number $q_{\rm cr}$ for which $\Theta(k_F, q_{\rm cr})$ (13) is equal to 1/2. In this case, x in Eq. (14) diverges, i.e. $q_{\rm cr}$ is the solution of the equation

$$\pi q_{\rm cr}^2 a_0 = -2k_F + (2k_F + q_{\rm cr}) \ln \frac{2k_F + q_{\rm cr}}{q_{\rm cr}}. \tag{22}$$

To summarize, for $q > q_{\rm cr}$, the energies of incoherent excitations are closer to their electron-hole counterparts than to the next neighboring electron-hole excitations, regardless to the value of the wave number $k_\parallel$. For $q < q_{\rm cr}$, the energies of incoherent excitations are closer either to their electron-hole counterparts or to the first larger neighboring electron-hole excitations for small and large values of the wave number $k_\parallel$, respectively. The wave number $q_{\rm cr}$ roughly separates these two regimes.

3. *Collective excitations*

In the above approximate calculations of energies of incoherent excitations, we explore the fact that corresponding zeros and poles of the dielectric function densely alternate on the ω-axis. However, this method cannot be used for the excitation with the highest energy, lying above the maximum of electron-hole excitation energy

$E(k_F,\boldsymbol{q})$ for a given $\boldsymbol{q}$. In order to determine the $\Omega(k_F,\boldsymbol{q})$-dependence of this collective mode, we write Eq. (1) in the form

$$\frac{\sum\limits_{k_\|=-k_F}^{k_F} g(k_\|,\boldsymbol{q})E(k_\|,\boldsymbol{q})\prod\limits_{k'_\|\neq k_\|}\Big[\omega^2-E^2(k'_\|,\boldsymbol{q})\Big]-(q^2L\pi/4e^2)\prod\limits_{k_\|=-k_F}^{k_F}\big[\omega^2-E^2(k_\|,\boldsymbol{q})\big]}{\prod\limits_{k_\|=-k_F}^{k_F}\big[\omega^2-E^2(k_\|,\boldsymbol{q})\big]}=0. \tag{23}$$

Factors that multiply the highest powers, $\omega^{k_FL\pi}$ and $\omega^{k_FL\pi-2}$ in the polynomial presentation of the nominator on the left-hand side are

$$a_{k_F}=-q^2L\pi/4e^2, \tag{24}$$

and
$$a_{k_F-2\pi/L}=\sum_{k_\|=-k_F}^{k_F} g(k_\|,\boldsymbol{q})E(k_\|,\boldsymbol{q})+\frac{q^2L\pi}{4e^2}\sum_{k_\|=-k_F}^{k_F} E^2(k_\|,\boldsymbol{q})\,, \tag{25}$$

respectively. As it follows from the elementary algebra, the ratio $a_{k_F-2\pi/L}/a_{k_F}$ is equal to the sum of all zeroes of Eq. (23). From this we get

$$\sum_{k=-k_F}^{k_F-2\pi/L}\Omega^2(k_\|,\boldsymbol{q})-E^2(k_\|,\boldsymbol{q})+\Omega^2(k_F,\boldsymbol{q})-E^2(k_F,\boldsymbol{q})=\omega_{\rm pl}^2\,. \tag{26}$$

The above relation is a sum rule which states that the sum of differences of the squares of excitation energies and corresponding electron-hole energies equals to the square of the plasmon energy $\omega_{\rm pl}^2=4\pi Ne^2/(L^3m)$ [1]. The dispersion of the collective mode $\Omega(k_F,\boldsymbol{q})\equiv\Omega_{\rm pl}(\boldsymbol{q})$ follows directly from this relation once the energies of the incoherent excitations are determined, as it was done in the previous section. To illustrate this, let us recall two characteristic points of the dispersion curve $\Omega_{\rm pl}(\boldsymbol{q})$. First, since all incoherent and electron-hole excitations vanish for $\boldsymbol{q}=0$, the above sum rule reproduces the well-known result that $\omega_{\rm pl}$ is the energy of the highest long-wavelength excitation, i. e. of the plasmon [1]. Second, it is known from the continuum approach [6] that the dispersion curve $\Omega_{\rm pl}(\boldsymbol{q})$ touches the border of the electron-hole continuum at a finite wave number. Here we point out that this wave number *coincides* with the wave number $q_{\rm cr}$ given by Eq. (22). The result by which plasmons do not exist as collective excitations at wave numbers at which all incoherent excitations are closer to their electron-hole counterparts than to the next neighboring electron-hole excitations can be derived in the following way. The plasmon dispersion $\Omega_{\rm pl}(\boldsymbol{q})$ follows also from Eq. (8) after omitting the term with poles and substituting $E(k_\|,\boldsymbol{q})$ by $\Omega_{\rm pl}(\boldsymbol{q})$ in the expression (9) for the function $F(k_\|,\boldsymbol{q})$. Thus we get

$$1-\frac{4}{\pi^2q^2a_0}F\left(\frac{m\Omega_{\rm pl}(\boldsymbol{q})}{q}-\frac{q}{2},\boldsymbol{q}\right)=0\,. \tag{27}$$

In the continuum approximation, the plasmon dispersion touches the border of the electron-hole quasi-continuum for $\Omega_{\rm pl}(\boldsymbol{q})=(2k_F+q)q/2m$. In this way, Eq.

(27) reduces to Eq. (22), i. e., the plasmon indeed ceases to exist as a collective excitation just at $q = q_{\rm cr}$.

In the original works [6] as well as in the textbooks [1, 2, 7–9], the touching point $q_{\rm cr}$ is usually interpreted as the wave number above which the decay of plasmons into electron-hole pairs takes part. Sometimes it is even stated or hinted that the dispersion curve $\Omega_{\rm pl}(\boldsymbol{q})$ and the upper border of electron-hole range cross at $q = q_{\rm cr}$ [2, 9]. We note that within the present discrete approach, the curve $\Omega_{\rm pl}(\boldsymbol{q})$ neither touches nor crosses the border of electron-hole excitations, but just approaches it at the distances of the order of $\Delta E(\boldsymbol{q})$, and remains at this distance for $q > q_{\rm cr}$. To show this quantitatively, let us calculate the highest excitation energy for $q \gg q_{\rm cr}$ by using the expression (21) for the differences $\Omega^2(k_\parallel, \boldsymbol{q}) - E^2(k_\parallel, \boldsymbol{q})$ in this limit. We get from the sum rule (26)

$$\Omega^2(k_F, q) - E^2(k_F, q) = \omega_{\rm pl}^2 - \frac{2e^2}{Lmq} \sum_{k_\parallel \neq k_F} \left(k_F^2 - k_\parallel^2\right)\left(2k_\parallel + q\right)\left[1 + \frac{4me^2 F(k_\parallel, \boldsymbol{q})}{\pi^2 q^2}\right]. \tag{28}$$

In order to calculate the sum on the right-hand side, we divide it in the convenient way and make the continuation,

$$\begin{aligned}\Omega^2(k_F, q) - E^2(k_F, q) \\ = \omega_{\rm pl}^2 - \frac{e^2}{\pi m q}\Bigg[\int_{-k_F}^{k_F} {\rm d}k\left(k_F^2 - k^2\right)(2k+q)\left[1 + \frac{4me^2 F(k_\parallel, \boldsymbol{q})}{\pi^2 q^2}\right] \\ - \int_{k_F - 2\pi/L}^{k_F} {\rm d}k\left(k_F^2 - k^2\right)(2k+q)\Bigg].\end{aligned} \tag{29}$$

After straightforward steps, we get

$$\Omega(k_F, q) = E(k_F, q) + \frac{e^2 k_F}{\pi q^2}\left(\frac{2\pi}{L}\right)^2, \tag{30}$$

noting that corrections to the energies of incoherent excitations as calculated in the previous section [introduced in Eq. (29) through the function $F(k_\parallel, \boldsymbol{q})$] do not contribute to the result (30) up to the order of $\omega_{\rm pl}^4/(q^6/m^3)$.

To conclude, the above analysis shows that the highest branch of excitations gradually approaches the quasi continuous incoherent electron-hole range as q approaches $q_{\rm cr}$ from below. In this range, it is a well-defined collective (plasmon) mode. For $q > q_{\rm cr}$, it remains above the top of this range at the microscopic energy difference of the order of $\Delta E(\boldsymbol{q})$ or less, and as such does not have the properties of a collective mode. Simultaneously as q passes through $q_{\rm cr}$ qualitative changes in the incoherent electron-hole range take place, as was already emphasized at the end of Sect. 2. In Fig. 2, we illustrate the above discussion, which to some extent complements that from Ref. [7], with numerical results for a large finite system. Note that our plasmon dispersion clearly differs from those schematically presented in, e.g., Refs.[2, 9].

We close this section with a short remark, based on the arguments given in Ref. [2], on the calculation of Im $\varepsilon(\boldsymbol{q}, \omega)$ in the present discrete approach. In order to get a proper result for the dissipative contributions to the correlation and response functions, one uses the standard recipe, i. e. calculates imaginary parts of their Fourier transforms only after the continuation in the reciprocal $\boldsymbol{q}$ - space. This order of steps is based on the assumption that the characteristic energetic level spacing in the system is sufficiently small in comparison to the reciprocal time of observation of the system. The equivalent proposition in the classical statistical physics is that the available time for the statistical averaging is much shorter than the Poincare cycle time. The duration of the time of observation, however, becomes irrelevant (i. e. it can be assumed arbitrarily long), once the continuation is performed.

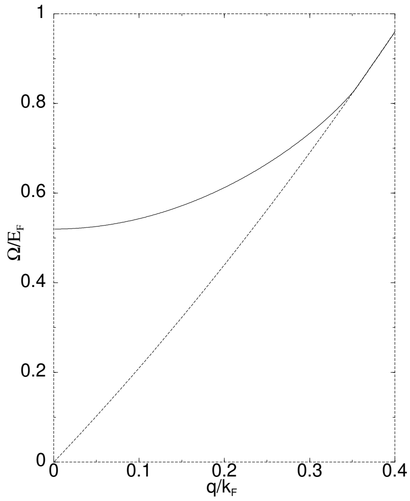

Fig. 2. The dispersion $\Omega(k_F, q)$ for $N = 8.37 \cdot 10^9$, and $L = 10a_0$. The asymptotic curve starting from origin is $E(k_F, q)$.

If one keeps, like in the present approach, the discrete summations throughout the calculations, the dissipative contributions are well-defined only after making averaging on the energy scales larger than the inherent energy level spacings. In particular, in our case one reproduces the correct result for Im $\varepsilon(\boldsymbol{q}, \omega)$ by averaging in ω on an interval not smaller than the energy differences $\Delta E(\boldsymbol{q})$ from Eq. (6). Indeed, after averaging the imaginary part of the dielectric function (1),

$$\mathrm{Im}\ \varepsilon(\boldsymbol{q}, \omega) = \frac{2e^2}{q^2 L} \sum_{k_\parallel = -k_F}^{k_F} g(k_\parallel, \boldsymbol{q}) \left\{ \delta\left[\omega + E(k_\parallel, \boldsymbol{q})\right] + \delta\left[\omega - E(k_\parallel, \boldsymbol{q})\right] \right\}, \qquad (31)$$

over $\Delta E(\boldsymbol{q})$, the smallest possible energy interval consistent with the above proposition, we get

$$\overline{\mathrm{Im}\ \varepsilon(\boldsymbol{q}, \omega)} = \frac{1}{\Delta E(\boldsymbol{q})} \int\limits_{\omega - \Delta E(\boldsymbol{q})/2}^{\omega + \Delta E(\boldsymbol{q})/2} \mathrm{Im}\ \varepsilon(\boldsymbol{q}, \omega') \mathrm{d}\omega' = \frac{me^2}{\pi q^3} g(\frac{m\omega}{q} - \frac{q}{2}, \boldsymbol{q}) \,. \qquad (32)$$

This is the well-known result for the imaginary part of the Lindhard function [1, 8, 9] in the region of the electron-hole quasi continuum. We note that the above averaging procedure might be particularly relevant for mesoscopic situations in which the cross-over from the dissipative regime to the regime without dissipation by varying the width of time (i.e., frequency) window becomes attainable experimentally.

4. Conclusion

In the standard treatments with continuous wave vector, the electron-hole region is reduced to a structureless continuum. The present analysis, in which we keep systematically the wave vector discreteness, leads to explicit results for shifts of energies of incoherent excitations with respect to the corresponding bare electron-hole excitation energies. Although these shifts are infinitesimal in macroscopic systems, their knowledge enables non-standard calculations of other physical observables, like correlation energies [4] and spectral functions [5]. The simple example of this kind is the calculation of the plasmon dispersion through the use of the sum rule (26).

The approach presented here may be straightforwardly extended to more complex macroscopic (e. g. multiband [4, 5]) systems. Furthermore, it is obviously particularly appropriate in studies of small mesoscopic systems in which electron-hole excitations are characterized by essentially larger energy level spacings with respect to those in the macroscopic limit. Then one also encounters interesting possibility of cross-over from the dissipatively irreversible to reversible regime, connected with fundamental principles of thermodynamic averaging.

Appendix

In this Appendix we consider the validity of the approximation introduced by passing from Eq. (1) to Eq. (8). By this step we replace in the residual sums [represented by the function $F(k_\parallel, \boldsymbol{q})$ (Eq. 12)] the exact value of a given solution $\Omega(k_\parallel, \boldsymbol{q})$ of Eq. (1) by the corresponding pole $E(k_\parallel, \boldsymbol{q})$ as defined by Eq. (7). Let us start from the exact expression for the function $F(k_\parallel, \boldsymbol{q})$

$$\begin{aligned}\tilde{F}(k_\parallel, q) = \frac{\pi}{mL}\Bigg[&\sum_{k'_\parallel=-k_F}^{k_\parallel-2\pi/L} \frac{g(k'_\parallel, q)E(k'_\parallel, q)}{\big[E(k_\parallel, q) + \Theta(k_\parallel, q)\Delta E(q)\big]^2 - E^2(k'_\parallel, q)} \\ &+ \sum_{k'_\parallel=k_\parallel+4\pi/L}^{k_F} \frac{g(k'_\parallel, q)E(k'_\parallel, q)}{\big[E(k_\parallel, q) + \Theta(k_\parallel, q)\Delta E(q)\big]^2 - E^2(k'_\parallel, q)}\Bigg].\end{aligned} \tag{33}$$

Here the value of the zero of Eq.(1) is written in the form (7). The Taylor expansion of $\tilde{F}(k_\parallel, \boldsymbol{q})$ in terms of $\Theta(k_\parallel, \boldsymbol{q})\Delta E(\boldsymbol{q})$ gives

$$\tilde{F}(k_\parallel, \boldsymbol{q}) - F(k_\parallel, \boldsymbol{q}) = F_1(k_\parallel, \boldsymbol{q})\Theta(k_\parallel, \boldsymbol{q})\Delta E(\boldsymbol{q}) + \mathcal{O}\left[[\Theta(k_\parallel, \boldsymbol{q})\Delta E(\boldsymbol{q})]^2\right], \tag{34}$$

with

$$F_1(k_\parallel,\boldsymbol{q}) = -\frac{2\pi}{mL}E(k_\parallel,\boldsymbol{q})\left[\sum_{k'_\parallel=-k_F}^{k_\parallel-2\pi/L}\frac{g(k'_\parallel,\boldsymbol{q})E(k'_\parallel,\boldsymbol{q})}{\left[E^2(k_\parallel,\boldsymbol{q})-E^2(k'_\parallel,\boldsymbol{q})\right]^2} + \sum_{k'_\parallel=k_\parallel+4\pi/L}^{k_F}\frac{g(k'_\parallel,\boldsymbol{q})E(k'_\parallel,\boldsymbol{q})}{\left[E^2(k_\parallel,\boldsymbol{q})^2-E^2(k'_\parallel,\boldsymbol{q})\right]^2}\right]. \tag{35}$$

This correction can be estimated after replacing sums by integrals. We get

$$F_1(k_\parallel,\boldsymbol{q}) = -\frac{g(k_\parallel,\boldsymbol{q})}{2q\Delta E(\boldsymbol{q})}. \tag{36}$$

The approximation is justified if

$$\left|\frac{F_1(k_\parallel,\boldsymbol{q})\Delta E(\boldsymbol{q})}{F(k_\parallel,\boldsymbol{q})}\right| = \frac{2g(k_\parallel,\boldsymbol{q})}{\pi\left|-2k_Fq-(k_F^2-k_\parallel^2)\ln\left|\frac{(k_F-k_\parallel)(k_F+k_\parallel+q)}{(k_F+k_\parallel)(k_F-k_\parallel-q)}\right|+(2k_\parallel+q)q\ln\left|\frac{k_F+k_\parallel+q}{k_F-k_\parallel-q}\right|\right|} \ll 1. \tag{37}$$

This condition is best fulfilled for small and large excitation energies due to the vanishing density of electron-hole excitations $g(k_\parallel,\boldsymbol{q})$. Eq. (37) also indicates that the approximation might be less adequate in the range of wave numbers k in which $F(k,\boldsymbol{q}) = 0$ is small. The value k_0 for which $F(k_0,\boldsymbol{q}) = 0$ can be determined

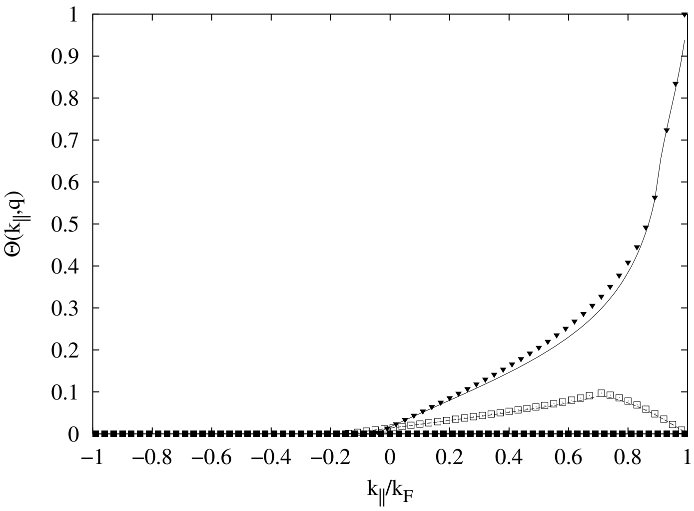

Fig. 3. The function $\Theta(k_\parallel,\boldsymbol{q})$ calculated by means of Eq. (13) (solid lines) and numerically from Eq. (1) for $k_F = 200\pi/L$, $L/a_0 = 10$ and for wave numbers $q = 0.1k_F$ (triangles), $0.3k_F$ (hollow squares) and $2k_F$ (filled squares).

from Eq. (12). Assuming $q \ll k_F - k_0$ we get

$$\frac{k_0}{k_F} \ln \frac{1 + \frac{k_0}{k_F}}{1 - \frac{k_0}{k_F}} \approx 1, \tag{38}$$

and $k_0 \approx 0.65 k_F$.

The direct insight into the validity of method follows from the comparison of analytically calculated values of differences $\Theta(k_\parallel, \boldsymbol{q}) = [\Omega(k_\parallel, \boldsymbol{q}) - E(k_\parallel \boldsymbol{q})]/\Delta E(\boldsymbol{q})$ and those obtained numerically for the mesoscopic system of $N \approx 8 \cdot 10^6 \pi/3$ electrons, and $L/a_0 = 10$, which by means of Eq. (22) gives $q_{\rm cr} \approx 0.13 k_F$. It is shown in Fig. 3. For $q = 0.1 k_F < q_{\rm cr}$ this difference raises monotonously from zero to unity, while for $q = 0.3 k_F > q_{\rm cr}$ it shows highly non monotonous behavior. Finally for $q = 2k_F >> q_{\rm cr}$ $\Theta(k_\parallel, \boldsymbol{q})$ is close to zero in the whole range of wave numbers $k_\parallel$. The curves in Fig. 3 clearly confirm the above estimations that the deviations of the results of analytic method from Sec. II from numerical calculations are negligible for small and large excitation energies. For intermediate values of excitation energies and for $q < q_{\rm cr}$ the method is less accurate, but deviations from numerical results are still quite small. Finally, for $q >> q_{\rm cr}$, this deviation is negligible for all excitations.

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DISKRETAN PRISTUP NEKOHERENTNIM UZBUDAMA U VODIČIMA

Računamo spektar nekoherentnih uzbuda elektron-šupljina u vodljivim Fermijevim tekućinama zadržavajući diskretnost recipročnog prostora. Pristup se predstavlja pomoću poznatog modela drhtavice i približenja nasumičnih faza. Dobiva se zbrojno pravilo iz kojeg slijede pojedinosti disperzijske krivulje za kolektivan plazmonski mod. Podsjeća se ukratko na pojam vremenskog prosjeka u ovom diskretnom pristupu.