Thermalized positrons in jellium: a GW investigation

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Abstract

Since many decades, positron annihilation experiments (lifetime, angular correlation, and Doppler broadening spectroscopy) play an important role for investigations of the electronic structure of both crystalline and amorphous materials. In this context, the *key quantity* to be studied is the momentum-dependent annihilation rate of electron-positron (e-p) pairs in electron gases. In this contribution, we present - at first time - a theory of annihilating e-p pairs in jellium where *both* the electron and positron propagators are treated on a GW level.

Introduction

The *momentum-dependent two-photon annihilation rate* of e-p pairs is given by [1]

$$R_{2\gamma}(\mathbf{p}) = 2\frac{r_0^2\pi c}{\Omega}\,\rho_{ep}(\mathbf{p})\,,$$

with r_0 and c as the classical electron radius and the velocity of light, and Ω as the volume of the system. $\rho_{ep}(\mathbf{p})$ means the *two-particle momentum density* of the annihilating pairs [2]

$$\rho_{ep}(\mathbf{p}) = -\int d^3x d^3y\, e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}\, G_{ep}(\mathbf{x}t,\mathbf{x}t;\mathbf{y}t^+,\mathbf{y}t^+)\,, \qquad (1)$$

where the first and the third arguments in the *two-particle electron-positron (ep) Green's function* G_{ep} belong to the electron and the second and forth arguments belong to the positron, respectively, and $t^+ - t$ means an infinitesimally small step forward in time.

$$G_{ep}(\mathbf{x}t,\mathbf{x}t;\mathbf{y}t^+,\mathbf{y}t^+) = G_e(\mathbf{x}t,\mathbf{y}t^+)\,G_p(\mathbf{x}t,\mathbf{y}t^+) + G^D_{ep}(\mathbf{x}t,\mathbf{x}t;\mathbf{y}t^+,\mathbf{y}t^+) \qquad (2)$$

reflects the physical situation of an e-p pair embedded in an electron gas: The first term, a product of the *one-particle* electron and positron Green's functions G_e and G_p, describes the two fermions interacting with the surrounding electrons but without taking into account any *direct* (D) interaction between the annihilating particles. These effects are treated by the second term of Eq. (2) and include all so-called *enhancement effects* of the e-p annihilation. In this paper, we focus our interest on the first term of Eq. (2) which is called the *independent-particle* (IP) approximation of the electron-positron Green's function:

$$G^{IP}_{ep}(\mathbf{x}t,\mathbf{x}t;\mathbf{y}t^+,\mathbf{y}t^+) = G_e(\mathbf{x}t,\mathbf{y}t^+)\,G_p(\mathbf{x}t,\mathbf{y}t^+)\,. \qquad (3)$$

In the case of a spatially and temporally *homogenous* electron gas (*jellium*), a combination of Eqs. (1) and (3) leads to

$$\rho^{IP}_{ep}(\mathbf{p}) = -\int d^3x d^3y\, e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}\, G_e(\mathbf{x}-\mathbf{y};t-t^+)\,G_p(\mathbf{x}-\mathbf{y};t-t^+)\,,$$

and after having Fourier-transformed $G(\mathbf{r},t) \to G(\mathbf{k},\omega)$, one obtains

$$\rho^{IP}_{ep}(\mathbf{p}) = \frac{(-i)^2}{(2\pi)^2}\sum_{\mathbf{k}}\int_{-\infty}^{+\infty} d\omega_1\, e^{i\omega_1\eta}\, G_e(\mathbf{k},\omega_1) \times \int_{-\infty}^{+\infty} d\omega_2\, e^{i\omega_2\eta}\, G_p(\mathbf{p}-\mathbf{k},\omega_2)\,, \qquad (4)$$

the momentum density of a system of N_- electrons and N_+ positrons with the corresponding Fermi radii

$$k_F^3 = 3\pi^2\frac{N_-}{\Omega} \quad \text{and} \quad (k_F^+)^3 = 3\pi^2\frac{N_+}{\Omega}\,. \qquad (5)$$

Now it is important to notice that, from the experimental point of view, one always has the situation

$$N_- >> N_+\,,$$

i.e., each positron is surrounded by a huge number of electrons, and there is no measurable interaction between the positrons. This situation of "one positron in N_- electrons". is taken into account by changing Eq. (4) into

$$\rho^{IP}_{ep}(\mathbf{p}) = \lim_{N_+\to 0}\frac{2}{N_+}\frac{(-i)^2}{(2\pi)^2}\sum_{\mathbf{k}}\int_{-\infty}^{+\infty} d\omega_1\, e^{i\omega_1\eta}\, G_e(\mathbf{k},\omega_1) \times \int_{-\infty}^{+\infty} d\omega_2\, e^{i\omega_2\eta}\, G_p(N_+;\mathbf{p}-\mathbf{k},\omega_2)\,. \qquad (6)$$

This equation describes the electron-positron momentum density *per positron* in the limit of an extremely small positron density.

Acknowledgments

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Electron Green's function

The electron one-particle Green's function G_e describes the propagation of an electron within the the surrounding electrons.

Due to the experimentally caused fact of $N_- << N_+$, the behavior of the electrons is not at all influenced by the positrons (the *direct interaction* between the annihilating partners is neglected in the IP model studied in this paper). Therefore, one has an unperturbed many-electron problem as it is intensively treated in the literature [3]: The Green's function including electron correlations is given by Dyson's formula [4]

$$G_e(\mathbf{k},\omega) = \frac{1}{\left[G^0_e(\mathbf{k},\omega)\right]^{-1} - \Sigma_e(\mathbf{k},\omega)} \qquad (7)$$

where G^0_e means the Green's function of the non-interacting particle

$$G^0_e(\mathbf{k},\omega) = \frac{\Theta(k_F-k)}{\omega-\omega^0_{\mathbf{k}}-i\eta} + \frac{\Theta(k-k_F)}{\omega-\omega^0_{\mathbf{k}}+i\eta} \qquad \text{with} \quad \omega^0_{\mathbf{k}} = \frac{\hbar k^2}{2m}\,.$$

Σ_e in Eq. (7) is the *electron self-energy function in the GW approximation* [4,5]

$$\hbar\Sigma_e^{(RPA)}(\mathbf{k},\omega) = \frac{i}{(2\pi)^4}\int d^3q\, V(\mathbf{q}) \times \int \frac{d\omega_1}{\kappa^{RPA}(\mathbf{q},\omega_1)}\, e^{i(\omega-\omega_1)\eta}\, G^0(\mathbf{k}-\mathbf{q},\omega-\omega_1)$$

where $V(\mathbf{q})$ means the Fourier coefficients of the bare Coulomb potential, and $\kappa^{RPA}(\mathbf{q},\omega_1)$ is the dielectric function of the electron gas in the *random phase approximation* (RPA) [4].

For the pure electronic system, the momentum distribution of the interacting electrons is then given by

$$\rho_e(\mathbf{k}) = \frac{1}{\pi}\int_{-\infty}^{\epsilon_F/\hbar} d\omega_1\, \frac{\Im\Sigma_e(\mathbf{k}\omega_1)}{\left[\omega_1-\omega^0_{\mathbf{k}}-\Re\Sigma_e(\mathbf{k},\omega_1)\right]^2 + \left[\Im\Sigma_e(\mathbf{k},\omega_1)\right]^2}\,. \qquad (8)$$

Corresponding results are shown in FIG. 1.

Positron occupation probability I

What concerns the role of the positron, we start with a combination of Eqs. (6) and (8) including the transformation $\mathbf{p}-\mathbf{k}\to\mathbf{q}$:

$$\rho^{IP}_{ep}(\mathbf{p}) = \lim_{N_+\to 0}\frac{2}{N_+}\sum_{\mathbf{q}}\rho_e(\mathbf{p}-\mathbf{q}) \times \left(\frac{-i}{2\pi}\right)\int_{-\infty}^{+\infty} d\omega_2\, e^{i\omega_2\eta}\, G_p(N_+;\mathbf{q},\omega_2)\,. \qquad (9)$$

Equivalent to the electron case, the integral over ω_2 reads as

$$\left(\frac{-i}{2\pi}\right)\int_{-\infty}^{+\infty} d\omega_2\, e^{i\omega_2\eta}\, G_p(N_+;\mathbf{k},\omega_1) = \frac{1}{\pi}\int_{-\infty}^{\epsilon_F^+/\hbar} d\omega_2\, \Im G_p(N_+;\mathbf{k},\omega_2)\,,$$

and using the relations (5) and $\epsilon_F^+/\hbar = \hbar(k_F^+)^2/(2m)$, Eq. (9) changes to

$$\rho^{IP}_{ep}(\mathbf{p}) = \frac{1}{4\pi}\int\frac{d^3q}{q^2}\,\rho_e(\mathbf{p}-\mathbf{q}) \times \left[\lim_{k_F^+\to 0}\frac{3q^2}{\pi(k_F^+)^3}\int_{-\infty}^{\hbar(k_F^+)^2/(2m)} d\omega_2\, \Im G_p(k_F^+;\mathbf{q},\omega_2)\right]$$

where $[\cdots]$ means *the radial occupation probability of a positron*

$$f^+(q) = \lim_{k_F^+\to 0}\frac{3q^2}{\pi(k_F^+)^3}\int_{-\infty}^{\hbar(k_F^+)^2/(2m)} d\omega_2 \times \frac{\Im\Sigma^+(k_F^+;q,\omega_2)}{\left[\omega_2-\omega^0_q-\Re\Sigma^+(k_F^+;q,\omega_2)\right]^2 + \left[\Im\Sigma^+(k_F^+;q,\omega_2)\right]^2}\,. \qquad (10)$$

The interaction of the positrons with the electron gas gives rise to a *probability tail* for $q \geq k_F^+$. By performing some non-trivial mathematical manipulations, it can be shown that this tail also exists in the limit $k_F^+\to 0$, leading to the relatively simple expression

$$f^+_{tail}(q) = -\frac{2e^2}{\hbar\pi^2}\int_{-\infty}^{0} d\omega\left(\Im\frac{1}{\kappa(q,-\omega)}\right) \times \left[\omega-\omega^0_q-\Re\Sigma^{+(c)}(0;q,\omega)\right]^{-2} \qquad (11)$$

with

$$\Re\Sigma^{+(c)}(0;q,\omega) = -\frac{e^2}{2\hbar\pi^3}\int\frac{d^3k}{k^2} \times \int_0^\infty d\sigma\left(\Im\frac{1}{\kappa(k,\sigma)}\right)\frac{1}{\omega-\sigma-\omega^0_{\mathbf{q}-\mathbf{k}}}\,.$$

Positron occupation probability II

The total occupation probability function reads as

$$f^+(q) = \nu^+\delta(q) + f^+_{tail}(q)\,, \qquad (12)$$

where ν^+ means the amplitude of the central delta distribution:

$$\nu^+ = 1 - \int_0^\infty dq\, f^+_{tail}(q)\,.$$

By combining Eqs. (8), (11) and (12), we are able to write down a compact formula for the independent-particle part of the electron-positron momentum density where both annihilation partners are GW described (see FIG.2 and FIG.3):

$$\rho^{IP}_{ep}(p) = \nu^+\rho_e(p) + \frac{1}{4\pi}\int\frac{d^3q}{q^2}\, f^+_{tail}(q)\,\rho_e(\mathbf{p}-\mathbf{q})\,. \qquad (13)$$

Results

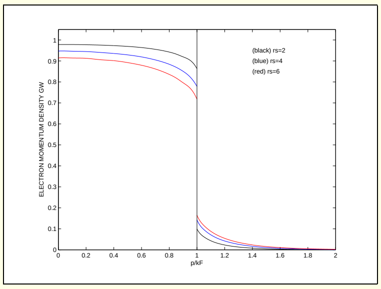

FIG. 1.: Electron momentum densities in jellium, calculated using a GW approximation.

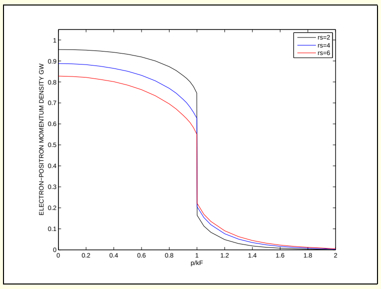

FIG. 2.: Electron-positron momentum densities in jellium in the IP approximation. Both the electron and the positron Green's functions are calculated according the GW approximation.

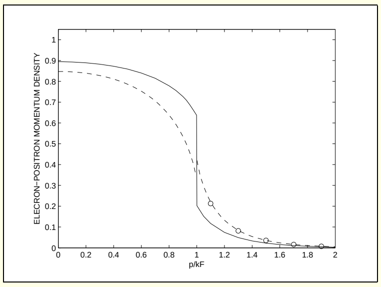

FIG. 3.: Electron-positron momentum-density in jellium (r_s=3.79) in the IP approximation. The solid line presents our new GW result based on Eq. (13), and the dashed line shows results obtained by performing a calculation of *first order* with respect of the electron and positron selfenergies. Such calculations have been done by Carbotte and Kahana (1965). Results from this paper are given as circles.

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