SCREENING OF THE COULOMB INTERACTION IN A GENERIC BALLISTIC QUANTUM DOT

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Abstract.
In semiconductor quantum dots, electrons behave as Fermi-Landau quasi-particles interacting through a week screened interaction. For confined systems a genuine "microscopic" derivation of how this screening takes place is made more complicated than in the bulk case because it has to be treated concurrently with the reorganization of charges generating the smooth electrostatic confining potential in which the electrons are evolving. This contribution gives a discussion of this problem in a semiclassical framework.

1. Introduction

Mesoscopic physics, in the sense of the study of small, fully coherent, electronic systems on the micron or sub-micron scale, is a field already a few decades old, with a significant number of achievements both experimental and theoretical (Sohn et al., 1997; Grabert and H. Devoret, 1992; Richter, 2000; Aleiner et al., 2002; Ullmo, 2008). The first experimental realizations of such mesoscopic systems were small metallic grains, for which the motion of the electrons within the sample is diffusive. Progress made in the patterning of two dimensional electron gas, in GaAs/AlGaAs or other kind of heterostructure, made it possible however since the early to produce and study ballistic quantum dots, for which the electrons motion is governed by the electrostatic confining potential.

In such systems, the interplay between Coulomb interaction $V_{\rm coul}(\mathbf{r},\mathbf{r}')$ and interference effects due to confinement plays, in many circumstances, a fundamental role. It is therefore somewhat surprising that, even at this time, there does not exist a proper theory of screening of the Coulomb interaction in ballistic quantum dots. For bulk (possibly disordered) electron gas, the mechanisms leading to screening are extremely well understood and have since long found their way into textbooks.

For finite systems, however an extra complication arises from the fact that screening takes place "together" with the reorganization of charges required to form the self consistent one body potential in which the electrons are evolving. Both processes (screening and and formation of the self consistent electrostatic potential) need to be treated concurrently, making significantly more involved a microscopic description.

In the semiclassical limit, and more precisely whenever the screening length κ^{-1} is much smaller than the typical size L of the system, a common wisdom approach is usually followed. This common wisdom simply states that since the characteristic scales of variation of the screened potential $V_{\rm sc}$ and of the electrostatic mean field potential $U_{\rm mf}$ are parametrically different (the former κ^{-1} is a quantum scale, when the latter L is classical), one could nevertheless use the same screened interaction as for the bulk, and furthermore assume that $U_{\rm mf}(\mathbf{r})$ is correctly approximated by a Thomas-Fermi approximation, which amount to solve the self consistent equation

$$U_{\rm mf}(\mathbf{r}) \;=\; U_{\rm ext}(\mathbf{r}) + \int \mathbf{dr'n(r')V}_{\rm coul}(\mathbf{r},\mathbf{r'}) \tag{1}$$

$$n(\mathbf{r}) \;=\; \int \frac{d\mathbf{p}}{(2\pi\hbar)^d}\Theta(\mu - U_{\rm mf}(\mathbf{r}) - \mathbf{p^2}/\mathbf{2m_e}) \; . \tag{2}$$

Interestingly enough, there is no general microscopic derivation of the above picture. More precisely, our confidence in having the Thomas-Fermi approximation as a correct starting point for the computation of $U_{\rm mf}$ is due to the fact that this approximation can be derived in a quite general framework starting from a density functional description (in e.g. the local density approximation) and neglecting the effect of interferences (Ullmo et al., 2001; Ullmo et al., 2004). The "common wisdom" prescription given above therefore essentially amounts to trusting the density functional approach on the classical scale L (although it might be less reliable on the quantum scale $\lambda_{\rm F}$; cf. for instance the discussion in (Ullmo et al., 2004)), keeping the usual (bulk) form of the screened interaction on the quantum scale, and assuming that the two scales are not going to interfere in any significant way.

There is a class of systems (namely billiards with weak disorder) for which it is possible to perform a renormalization procedure (Blanter et al., 1997; Aleiner et al., 2002) where the fast modes are integrated out so that only the interesting low-energy physics remains. It is then possible to see how both the mean field and the screened interaction emerge in that case from this procedure.

Ideally, the aim of this contribution should have been to generalize this renormalization approach to a generic ballistic quantum dot. This

appears out of reach at the present time, and I will limit myself here to a significantly more modest goal, namely to investigate how far the approach introduced in section 2.3.2 of (Aleiner et al., 2002) can be generalized to the case of a generic quantum dot (i.e. one for which $U_{\rm mf}(\mathbf{r})$ is not well approximated by a constant), but also to identify the main difficulty preventing a full solution of the problem. I hope this will provide some useful milestone in the solution of this problem in the ballistic case, as well as indicate some possible limitations existing already in the diffusive one.

2. renormalization scheme

In the bulk, the RPA screened interaction, is obtained by considering the Dyson equation for the dressed interaction (see the discussion in section 9 of Fetter and Walecka (Fetter and Walecka, 1971))

$$V_{\rm dressed}(\mathbf{r_1},\mathbf{r_2},\omega) = V_{\rm coul}(\mathbf{r_1}-\mathbf{r_2}) + \int d\mathbf{r}\int \mathbf{dr'}\mathbf{V}_{\rm coul}(\mathbf{r_1}-\mathbf{r})\mathbf{\Pi}(\mathbf{r},\mathbf{r'},\omega)\mathbf{V}_{\rm dressed}(\mathbf{r'},\mathbf{r_2},\omega)\ , \tag{3}$$

which is exact if all the one-particle irreducible diagrams are included for the polarization operator Π but gives the RPA approximation if only the (lowest order) bubble diagram

$$\Pi^0(\mathbf{r},\mathbf{r'},\omega) = \mathrm{g_s}\int_{-\infty}^{+\infty}\frac{\mathbf{d}\omega'}{\mathbf{2i}\pi}\mathbf{G}(\mathbf{r},\mathbf{r'},\omega+\omega')\mathbf{G}(\mathbf{r'},\mathbf{r},\omega') \tag{4}$$

is kept. $G(\mathbf{r},\mathbf{r'},\omega) = \mathbf{\Theta}(\omega)\mathbf{G^R}(\mathbf{r},\mathbf{r'},\omega) + \mathbf{\Theta}(-\omega)\mathbf{G^A}(\mathbf{r},\mathbf{r'},\omega)$ is the unperturbed time ordered Green's function, with $\Theta(x)$ the Heaviside function, and $\mathrm{g_s} = 2$ is the spin degeneracy factor. In the zero frequency low momentum limit one gets (in the bulk) $\Pi^0(\mathbf{r},\mathbf{r'},\omega=\mathbf{0}) \simeq -\mathrm{g_s}\nu_\mathbf{0}\delta(\mathbf{r}-\mathbf{r'})$, with ν_0 the local density of states per spin. Inserting this expression for Π^0 in (3) gives the low momentum zero frequency RPA approximation of the screened interaction.

Let us consider now a mesoscopic systems, and assume that its typical dimensions are much larger than the screening length. One then expects that the residual screened Coulomb interaction should be very similar to the one in the bulk, and it is therefore natural to approach the question from the same viewpoint. In that case however the Green's function are not known exactly, so one needs to resort to semiclassical approximations of $G^{R,A}$ in the expression of Π^0. The difficulty encountered then is that semiclassical approximations are valid

for high energies (high ω), and in particular one cannot expect the semiclassical expressions for $G(\mathbf{r},\mathbf{r}',\omega)$ to be accurate if ω is not much larger than the mean level spacing Δ of the system.

Following (Aleiner et al., 2002), the idea is then, in the spirit of the renormalization group approach, to integrate out only the "fast variable" (high-energy part) for which a semiclassical approximations can be used, and to deal with the low energy physics by some other methods (based for instance on a random-matrix description (Murthy and Mathur, 2002; Murthy and Shankar, 2003)). Using the exact expression for the polarization bubble

$$\Pi^0(\mathbf{r},\mathbf{r}',\omega) = \mathrm{g_s}\sum_{\mathbf{n}\mathbf{n}'}\mathbf{\Theta}(-\epsilon_{\mathbf{n}}\epsilon_{\mathbf{n}'})\frac{\varphi^*_{\mathbf{n}}(\mathbf{r}')\varphi_{\mathbf{n}}(\mathbf{r})\varphi^*_{\mathbf{n}'}(\mathbf{r})\varphi_{\mathbf{n}'}(\mathbf{r}')}{\omega+\epsilon_{\mathbf{n}'}-\epsilon_{\mathbf{n}}}(-\mathrm{sgn}(\epsilon_{\mathbf{n}})) \tag{5}$$

with $(\epsilon_n,\varphi_n(\mathbf{r}))$ the one-particle energies and eigenstates, we see that this can be achieved by restricting the sum in the above expression to pair (n,n') such that at least one energy is outside a band centered at the Fermi energy ϵ_F (taken as the origin of energies) and of width ϵ^* chosen such that $\Delta \ll \epsilon^* \ll E_{\mathrm{Th}}$, and which precise value (once in this range) is expected to be irrelevant. Up to an unimportant boundary term, this is equivalent to restricting the sum to particle-hole energies $\epsilon_{n'}-\epsilon_n$ larger (in absolute value) than ϵ^*. Introducing $\Pi^{R,A}(\mathbf{r},\mathbf{r}',\omega) \stackrel{\mathrm{def}}{=} \lim_{\eta\to\mathbf{0}+}\mathbf{\Pi^0}(\mathbf{r},\mathbf{r}',\omega\pm\mathbf{i}\eta)$ the retarded and advance polarization bubbles, one can therefore write the polarization operator in which only the fast modes are integrated out as

$$\hat{\Pi}_{\epsilon^*}(\mathbf{r}',\mathbf{r},\tilde{\omega}=\mathbf{0}) = \frac{\mathbf{1}}{\mathbf{2i}\pi}\int\frac{\mathbf{d}\omega}{\omega}\left[\mathbf{\Pi^R}(\mathbf{r},\mathbf{r}',\omega)-\mathbf{\Pi^A}(\mathbf{r},\mathbf{r}',\omega)\right]\mathbf{\Theta}(|\omega|-\epsilon^*)\ . \tag{6}$$

The insertion of $\hat{\Pi}_{\epsilon^*}$ in (3) will then give the effective interaction describing the low energy ($\leq\epsilon^*$) physics of the quantum dot.

3. Calculation of the polarization loop

Let us first consider positive energies $\omega>0$. Noting that phase cancellation is possible only for the product G^AG^R, but not for G^RG^R or G^AG^A, one has

$$\Pi^R(\mathbf{r},\mathbf{r}',\omega) = \mathrm{g_s}\int_{-\omega}^{\mathbf{0}}\frac{\mathbf{d}\omega'}{\mathbf{2i}\pi}\mathbf{G^R}(\mathbf{r},\mathbf{r}',\omega'+\omega+\mathbf{i}\eta)\mathbf{G^A}(\mathbf{r}',\mathbf{r},\omega') \tag{7}$$

and

$$\Pi^A(\mathbf{r},\mathbf{r}',\omega) = \mathbf{\Pi^R}(\mathbf{r}',\mathbf{r},\omega)^*\ . \tag{8}$$

The Green's functions in the l.h.s of Eq. (7) can be evaluated semiclassically as a sum over classical trajectories (Gutzwiller, 1990)

$$G^R(\mathbf{r},\mathbf{r}';\epsilon) \simeq \sum_{j:\mathbf{r}'\to\mathbf{r}} G_j^R(\mathbf{r},\mathbf{r}';\epsilon)$$
$$G_j^R(\mathbf{r},\mathbf{r}';\epsilon) \stackrel{\text{def}}{=} \frac{2\pi}{(2i\pi\hbar)^{(d+1)/2}} D_j(\epsilon)\exp\left(iS_j(\epsilon)/\hbar - i\zeta_j\pi/2\right) , \quad (9)$$

with S_j the classical action of the trajectory j going from $\mathbf{r}'$ to $\mathbf{r}$, ζ_j is a Maslov index, and the determinant D_j is a measure of the stability of the orbit. Keeping only the diagonal approximation in which a trajectory j is paired with itself to cancel the oscillating phases, one gets

$$[G^R(\mathbf{r},\mathbf{r}',\omega+\omega')\mathbf{G}^{\mathbf{A}}(\mathbf{r}',\mathbf{r},\omega')]_{\text{diag}} = \quad (10)$$
$$\sum_{j:\mathbf{r}\to\mathbf{r}'} \frac{4\pi^2}{(2\pi\hbar)^{d+1}}|D_j|^2\exp\left[i(S_j(\omega+\omega')-S_j(\omega'))/\hbar\right] .$$

In this equation, one would like then to perform a Taylor expansion of the action

$$(S_j(\omega+\omega')-S_j(\omega')) = (\partial S_j/\partial\epsilon)\omega = t_j\omega . \quad (11)$$

Inserting the unity $\int_0^\infty \delta(t-t_j)$ and making use of the sum rule (Argaman, 1996)

$$\sum_{j:\mathbf{r}'\to\mathbf{r}} \frac{|D_j(\epsilon)|^2}{(2\pi\hbar)^d}\delta(t-t_j) = \nu_0^{(d)}(\mathbf{r}')\mathbf{P}_{\text{cl}}^{\epsilon}(\mathbf{r},\mathbf{r}',\mathbf{t}) , \quad (12)$$

where $\nu_0^{(d)}(\mathbf{r}')$ is the bulk density of states per unit area (and spin) for the local value of k_F and $P_{\text{cl}}^{\epsilon}(\mathbf{r},\mathbf{r}',\mathbf{t})$ is the classical (density of) probability that a trajectory launched in $\mathbf{r}'$ is in the neighborhood of $\mathbf{r}$ at time t, we obtain

$$[G^R(\mathbf{r},\mathbf{r}',\omega+\omega')\mathbf{G}^{\mathbf{A}}(\mathbf{r}',\mathbf{r},\omega')]_{\text{diag}}$$
$$= \frac{4\pi^2}{(2\pi\hbar)^{d+1}}\int_0^\infty dt \sum_{j:\mathbf{r}\to\mathbf{r}'}|D_j|^2\delta(t-t_j)\exp\left[it\omega/\hbar\right] \quad (13)$$
$$= \frac{2\pi\nu_0(\mathbf{r}')}{\hbar}\int_0^\infty dt P_{\text{cl}}^{\epsilon}(\mathbf{r},\mathbf{r}',\mathbf{t})\exp\left[\mathbf{it}\omega/\hbar\right] \quad (14)$$
$$= 2\pi\nu_0(\mathbf{r})\hat{\mathbf{P}}_{\text{cl}}^{\epsilon}(\mathbf{r},\mathbf{r}',\omega) , \quad (15)$$

with $P^{\epsilon}_{\rm cl}$ the Fourier transform of the classical probability $P^{\epsilon}_{\rm cl}$. Interestingly enough $[G^R(\omega+\omega')G^A(\omega')]_{\rm diag}$ is independent of ω', so that finally

$$\Pi^R(\mathbf{r},\mathbf{r}',\omega) = -\mathbf{i}\omega \mathrm{g_s}\nu_{\mathbf{0}}(\mathbf{r}')\hat{\mathbf{P}}^{\epsilon}_{\rm cl}(\mathbf{r},\mathbf{r}',\omega)\ . \tag{16}$$

Note that the fact that we have computed Π^R, i.e. that $\omega \equiv \omega + i\eta$, is what is making the Fourier transform in (14) convergent. If we had computed Π^A the above approach would have lead to divergences. Π^A should therefore be derived from Π^R using (8), giving

$$\Pi^A(\mathbf{r},\mathbf{r}',\omega) = \mathbf{i}\omega \mathrm{g_s}\nu_{\mathbf{0}}(\mathbf{r})\hat{\mathbf{P}}^{\epsilon}_{\rm cl}(\mathbf{r}',\mathbf{r},\omega)\ . \tag{17}$$

For negative ω, Π^A should be calculated first and Π^R derived from it with (8), leading to the same result.

Here, one rather important remark is in order. The expression (11) assumes obviously that ω is small. This is usually not a significant constraint since the actions S_i are classical quantities, so that the relevant scale is the Fermi energy (or bandwidth) ϵ_F. It is therefore enough that $\omega \ll \epsilon_F$ to apply (11). However the integral in the left hand side of (6) is not limited to the neighborhood of the Fermi surface. Replacing $\Pi^{R,A}$ by the approximations (16)-(17) will be incorrect on the edge of the energy band, which will be associated to short distances $|\mathbf{r}-\mathbf{r}'| < \lambda_{\rm F}$. This will be the cause of the problems we shall encounter later on. Let us ignore this issue for the time being, and come back to this discussion when it will become obvious that the results obtained in this way are unphysical.

Then, inserting (16)-(17) into (6) and writing $\Theta(x) = 1 - \Theta(-x)$ we get

$$\hat{\Pi}_{\epsilon^*}(\mathbf{r}',\mathbf{r},\tilde{\omega}=\mathbf{0}) = -\mathrm{g_s}\int_{-\infty}^{+\infty}\frac{\mathbf{d}\omega}{\mathbf{2}\pi}\left[\nu_{\mathbf{0}}(\mathbf{r}')\tilde{\mathbf{P}}^{\epsilon}_{\rm cl}(\mathbf{r},\mathbf{r}',\omega)+\nu_{\mathbf{0}}(\mathbf{r})\tilde{\mathbf{P}}^{\epsilon}_{\rm cl}(\mathbf{r},\mathbf{r}',\omega)\right] \times(1-\Theta(\epsilon^*-|\omega|))\ . \tag{18}$$

The term proportional to one in the integrand of (18) gives rise to $\int(d\omega/2\pi)\tilde{P}^{\epsilon}_{\rm cl}(\mathbf{r},\mathbf{r}',\omega) = \mathbf{P}^{\epsilon}_{\rm cl}(\mathbf{r},\mathbf{r}',\mathbf{t}=\mathbf{=}\,\mathbf{0})$. To evaluate the remaining term, it is useful to discuss the weight function $\Theta(\epsilon^*-|\omega|)$. Its precise form is irrelevant here, and, rather than the actual Heaviside step function, I shall assume that $\Theta(\epsilon^*-|\omega|)$ is actually a smooth function $\Theta_{\epsilon^*}(\omega)$ which is zero for $|\omega| \gg \epsilon^*$ and one for $|\omega| \ll \epsilon^*$. To fix the idea one can think for instance of $\Theta_{\epsilon^*}(\omega) = \exp(-(1/2)(\omega/\epsilon^*)^2)$, but this precise form will not play any particular role. If one introduces $\tilde{\Theta}_{\epsilon^*}(t)$ the Fourier transform of $\Theta_{\epsilon^*}(\omega)$, one has, with $t^* = \hbar/\epsilon^*$

$$\tilde{\Theta}_{\epsilon^*}(t)\ \simeq\ 1/t^* \qquad \text{for } t \ll t^* \tag{19}$$

$$= 0 \qquad \text{for } t \gg t^* \tag{20}$$

$$\int_0^\infty dt\, \tilde{\Theta}_{\epsilon^*}(t) = \Theta_{\epsilon^*}(\omega = 0) = 1\ . \tag{21}$$

Assuming furthermore that $\tilde{\Theta}_{\epsilon^*}(t)$ is a positive function (this hypothesis can be easily relaxed), we see that $\tilde{\Theta}_{\epsilon^*}(t)$ is a density probability (since it is positive and normalized to one) which selects trajectory shorter than t^*. We thus can write

$$\hat{\Pi}_{\epsilon^*}(\mathbf{r}', \mathbf{r}, \tilde{\omega}=\mathbf{0}) = -\mathrm{g_s}\left[\nu_{\mathbf{0}}(\mathbf{r}')\mathbf{P}^{\epsilon}_{\mathrm{cl}}(\mathbf{r}, \mathbf{r}', \mathbf{t}=\mathbf{0})\right. \tag{22}$$
$$\left. -\frac{1}{2}\left(\nu_0(\mathbf{r}')\langle \mathbf{P}^{\epsilon}_{\mathrm{cl}}(\mathbf{r}, \mathbf{r}', \mathbf{t})\rangle_{\mathbf{t}\leq\mathbf{t}^*} + \nu_{\mathbf{0}}(\mathbf{r})\langle \mathbf{P}^{\epsilon}_{\mathrm{cl}}(\mathbf{r}', \mathbf{r}, \mathbf{t})\rangle_{\mathbf{t}\leq\mathbf{t}^*}\right)\right]\ ,$$

where $\langle f(t)\rangle_{t\leq t^*} \stackrel{\mathrm{def}}{=} \int_0^\infty dt\, f(t)\tilde{\Theta}_{\epsilon^*}(t)$ is the average over time t lesser than t^* of the function $f(t)$.

Now $P^{\epsilon}_{\mathrm{cl}}(\mathbf{r}, \mathbf{r}', \mathbf{t} = \mathbf{0}) = \delta(\mathbf{r} - \mathbf{r}')$. Furthermore, the condition $\Delta \ll \epsilon^* \ll E_{\mathrm{Th}}$ is equivalent to $t_f \ll t^* \ll t_H$, with $t_H = \hbar/\Delta$ the Heisenberg time and t_f the time of flight across the system (for ballistic systems) or time needed to diffuse to the boundary (for diffusive systems). We see that the choice of ϵ^* is made precisely so that i) semiclassical approximations are valid, but also ii) that most of the range $[0, t^*]$ is such that *for diffusive or chaotic systems* (the case of integrable or mixed system should be investigated in this respect), the motion can be assumed randomized. Assuming ergodicity we can therefore write

$$\langle P^{\epsilon}_{\mathrm{cl}}(\mathbf{r}, \mathbf{r}', \mathbf{t})\rangle_{\mathbf{t}\leq\mathbf{t}^*} \simeq \frac{\int \mathbf{dp}\delta(\epsilon_{\mathbf{F}} - \mathbf{H}(\mathbf{r}, \mathbf{p}))}{\int \mathbf{dr}''\mathbf{dp}''\delta(\epsilon_{\mathbf{F}} - \mathbf{H}(\mathbf{r}'', \mathbf{p}''))} = \mathbf{\Delta}\nu_{\mathbf{0}}(\mathbf{r})\ . \tag{23}$$

This eventually leads to

$$\hat{\Pi}_{\epsilon^*}(\mathbf{r}', \mathbf{r}, \tilde{\omega}=\mathbf{0}) = -\mathrm{g_s}\left[\nu_{\mathbf{0}}(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}') - \nu_{\mathbf{0}}(\mathbf{r})\nu_{\mathbf{0}}(\mathbf{r}')\mathbf{\Delta}\right]\ , \tag{24}$$

where one recognize the first term as the zero frequency low momentum bulk polarization$\Pi^0_{\mathrm{bulk}}(\mathbf{r}', \mathbf{r}, \tilde{\omega} = \mathbf{0}) = -\mathrm{g_s}\nu_{\mathbf{0}}(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}')$, and I will denote by

$$\Pi_{l.r.} \stackrel{\mathrm{def}}{=} \mathrm{g_s}\nu_0(\mathbf{r})\nu_{\mathbf{0}}(\mathbf{r}')\mathbf{\Delta} \tag{25}$$

the remaining long range part. For billiard systems for which $\nu_0(\mathbf{r}) = (\mathcal{A}\mathbf{\Delta})^{-\mathbf{1}} = \mathrm{const.}$, with $\mathcal{A}$ the volume of the system, (24) is for instance exactly the equation (60) of (Aleiner et al., 2002).

4. Self-consistent equation

In the bulk, both the Coulomb interaction and the polarization operator $\Pi^0_{\rm bulk}$ are translation invariant and the Dyson equation (3) can be solved in momentum representation as

$$\hat{V}_{\rm dressed}(\mathbf{q}) = \frac{\hat{\mathbf{V}}_{\rm coul}(\mathbf{q})}{\mathbf{1} - \hat{\mathbf{V}}_{\rm coul}(\mathbf{q})\hat{\mathbf{\Pi}}^{\mathbf{0}}_{\rm bulk}(\mathbf{q})} \ . \tag{26}$$

The resulting interaction is then short range, effectively much weaker than the original Coulomb interaction, and is therefore well adapted for a perturbative treatment.

The difficulty one encounters in the mesoscopic case is twofold. First, lack of translational invariance for Π_{ϵ^*} makes in principle (3) impossible to be solved in closed form for a generic spatial variations of $\nu_0(\mathbf{r})$. Second, we know that even at the level of electrostatics, the effects of the interactions cannot be small since they will at minima rearrange considerably the static charges within the system. Therefore, even if (3) could be solved, there is little chance that the resulting dressed interaction could be effectively used in a perturbative approach starting from the non-interacting electrons Hamiltonian.

For a quantum dot with a fixed number $(N+1)$ of electrons, one way to solve both of these difficulties is to derive a self-consistent equation following one of the standard derivation of the Hartree Fock approximation (Thouless, 1961). For this purpose, let us note that any one-body potential $\tilde{U}(\mathbf{r})$, can be written formally as the two-body interaction

$$\tilde{V}(\mathbf{r},\mathbf{r}') = \frac{\mathbf{1}}{\mathbf{N}}(\tilde{\mathbf{U}}(\mathbf{r}) + \tilde{\mathbf{U}}(\mathbf{r}')) \tag{27}$$

since, using for instance a second quantization formalism

$$\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\hat{\mathbf{\Psi}}^\dagger(\mathbf{r})\hat{\mathbf{\Psi}}^\dagger(\mathbf{r}')\tilde{\mathbf{V}}(\mathbf{r},\mathbf{r}')\hat{\mathbf{\Psi}}(\mathbf{r}')\hat{\mathbf{\Psi}}(\mathbf{r}) = \int \mathbf{r}\hat{\mathbf{\Psi}}^\dagger(\mathbf{r})\tilde{\mathbf{U}}(\mathbf{r})\hat{\mathbf{\Psi}}(\mathbf{r}) \ . \tag{28}$$

As a consequence, the total Hamiltonian, as well as the formalism presented in the first part of this contribution, are unmodified if the confining potential $U_{\rm ext}(\mathbf{r})$ and the Coulomb potential $V_{\rm coul}(\mathbf{r},\mathbf{r}')$ are respectively replaced by

$$U(\mathbf{r}) \ = \ U_{\rm ext}(\mathbf{r}) + \tilde{\mathbf{U}}_(\mathbf{r}) \tag{29}$$

$$V(\mathbf{r},\mathbf{r}') \ = \ V_{\rm coul}(\mathbf{r},\mathbf{r}') - \tilde{\mathbf{V}}(\mathbf{r},\mathbf{r}') \tag{30}$$

One can then now use the freedom in the choice of the function $\tilde{U}(\mathbf{r})$ to simplify the Dyson equation. In particular, if we can impose that

$$\int d\mathbf{r} \int \mathbf{dr'V}(\mathbf{r_1},\mathbf{r})\mathbf{\Pi}_{\rm l.r.}(\mathbf{r},\mathbf{r'})\mathbf{V}_{\rm dressed}(\mathbf{r'},\mathbf{r_2}) \equiv \mathbf{0} \ , \tag{31}$$

the Dyson equation (3) would then have the usual "bulk-like" form

$$V_{\rm dressed}(\mathbf{r_1},\mathbf{r_2}) = \mathbf{V}(\mathbf{r_1},\mathbf{r_2}) - \int \mathbf{dr} \int \mathbf{dr'V}(\mathbf{r_1},\mathbf{r})\mathbf{\Pi}^{\mathbf{0}}_{\rm bulk}(\mathbf{r}-\mathbf{r'})\mathbf{V}_{\rm dressed}(\mathbf{r'},\mathbf{r_2}) \ , \tag{32}$$

which, if $\nu_0(\mathbf{r})$ and $\tilde{U}(\mathbf{r})$ vary slowly on the scale of the bulk screening length κ^{-1} has the same solution as in the bulk.

Now, equation (31) might seem at first sight difficult to solve since it involves the unknown function $V_{\rm dressed}(\mathbf{r'},\mathbf{r_2})$. However, since $\Pi_{\rm l.r.}(\mathbf{r},\mathbf{r'})$ does actually not correlate $\mathbf{r}$ and $\mathbf{r'}$, the two integrals in (31) actually decouple, and a sufficient condition to solve this equation is that $\int d\mathbf{r}\mathbf{V}(\mathbf{r_1}-\mathbf{r})\nu(\mathbf{r}) \equiv \mathbf{0}$, i.e.

$$\int d\mathbf{r}\mathbf{V}_{\rm coul}(\mathbf{r_1}-\mathbf{r})\nu(\mathbf{r}) = \frac{\mathbf{1}}{\mathbf{N}} \int \mathbf{dr}\nu(\mathbf{r})(\tilde{\mathbf{U}}(\mathbf{r}) + \tilde{\mathbf{U}}(\mathbf{r_1})) \ . \tag{33}$$

The constant term $\int d\mathbf{r}\nu(\mathbf{r})\tilde{\mathbf{U}}(\mathbf{r})/\mathbf{N}$ is irrelevant here as it can be eliminated by a constant shift of $\tilde{U}$. One therefore obtain in this way the self-consistent equation

$$\tilde{U}(\mathbf{r_1}) = \mathbf{N\Delta} \int \mathbf{dr}\mathbf{V}_{\rm coul}(\mathbf{r_1}-\mathbf{r})\nu(\mathbf{r}) \ . \tag{34}$$

In other words what we have obtained for the self-consistent potential are the equations

$$U_{\rm mf}(\mathbf{r}) \ = \ U_{\rm ext}(\mathbf{r}) + \tilde{\mathbf{N}}\mathbf{\Delta} \int \mathbf{dr'}\nu_{\mathbf{0}}(\mathbf{r'})\mathbf{V}_{\rm coul}(\mathbf{r},\mathbf{r'}) \tag{35}$$

$$\nu_0(\mathbf{r}) \ = \ \int \frac{d\mathbf{p}}{(2\pi\hbar)^d}\delta(\mu - U_{\rm mf}(\mathbf{r}) - \mathbf{p^2/2m}) \ . \tag{36}$$

5. Discussion and Conclusion

The above result looks very much like what we expected to obtain as we began this discussion. Indeed Eqs. (32), (35) and (36), express than integrating out the "fast degree of freedom" allows one to separate in a natural way the screened potential in two parts: a first one which is a one body potential determined self consistently, and a second which

is just the usual bulk screened interaction with the local parameters of the electron gas (provided that $\tilde{U}(\mathbf{r})$ (and thus $\tilde{V}(\mathbf{r},\mathbf{r}')$) varies slowly on the scale of the screening length).

What makes this description less useful however is the self consistent Eqs. (35)-(36) are obviously incorrect. Indeed we know that whatever self-consistent equations we end up writing, they should contain in some approximation the electrostatic equilibrium of the problem. This is not the case here. If the self-consistent potential $U_{\mathrm{mf}}(\mathbf{r}) \stackrel{\mathrm{def}}{=} \mathbf{U}_{\mathrm{ext}}(\mathbf{r}) + \tilde{\mathbf{U}}(\mathbf{r})$ obtained from (34) is well approximated by a constant (giving for instance a billiard system with weak disorder as was considered in (Blanter et al., 1997) and (Aleiner et al., 2002)), and assuming $(N+1) \gg 1$, one can perform the replacement $N\Delta\nu(\mathbf{r}) \to \mathbf{n}(\mathbf{r})$ in (34) and write instead

$$\tilde{U}(\mathbf{r_1}) = \int \mathbf{dr} \mathbf{V}_{\mathrm{coul}}(\mathbf{r_1} - \mathbf{r}) \mathbf{n}(\mathbf{r}) \; , \tag{37}$$

i.e. (1)-(2), which is just the Thomas Fermi equation, from which plain electrostatic is obtained by neglecting the kinetic energy associated to Pauli exclusion principle. However for a generic confining potential $U_{\mathrm{ext}}(\mathbf{r})$, solutions of (34) will not in general be an approximation of the solution of (37).

To identify why we ended up with an incorrect equation is actually not very difficult. Indeed, the symptom is that the expected density of particle $n(\mathbf{r})$ has been replaced in Eq. (34) by the $N\nu(\mathbf{r})$, i.e. an extrapolation of what is going on near the Fermi energy. What we see is that, in some sense, equation (34) is "aware" of the properties of the system near the Fermi energy (the density of states $\nu(\mathbf{r})$), but misses the relevant information at large energies, of the order of the bandwidth, which determine the actual density of particles. This is to be expected since our approximation of the polarization operator Π^*_ϵ (24) involves only the local density of states at the Fermi energy $\nu(\mathbf{r})$. Going further back we see that in the end this behavior can be tracked back to the approximation (11) where the action $S(\omega)$ has been linearized near the Fermi energy, eliminating in this way any information relevant to the large (i.e. $\omega \sim \epsilon_F$) energies.

In the end, what makes non trivial the discussion of screening in a finite system is that the renormalization procedure which transform the bare Coulomb interaction into the screened one should also describe the emergence of the electrostatic mean field. When the former is essentially dominated by the neighborhood of the Fermi energy, the latter requires an accurate description of the physics at the band edge.

To conclude, and since obviously this contribution do not provide a satisfactory solution of the issue of screening in closed quantum dot, a few word about its possible usefulness in presumably warranted. The necessity to treat concurrently different energy scales is what is making non-trivial the problem at hand, but the corresponding separation of scale is however what sort of guarantee that the "common wisdom" approach of the screening described in the introduction is at least qualitatively correct. This common wisdom approach is moreover presumably sufficient as far as qualitative or statistical descriptions are concerned. The absence of a proper microscopic understanding of screening for closed system might however become a limitation when accurate simulation tools are required to describe quantitatively the particular behavior of a specific mesoscopic system. This is particularly true in the view of the fact that standard self consistent approaches, such as density functional theory calculations, fail to describe some of their important aspects (Ullmo et al., 2004). I hope this contribution, by identifying an essential conceptual difficulty in an approach which seems to get us extremely close to the expected result, will provide a useful step toward its full resolution. Moreover, as it turns out that it is not the diffusive character of the dynamics, but rather the possibility to extrapolated the local density of state up to the band edge which turn out to be the relevant difficulty here, it might also indicate some limitation of results derived in the more traditional context diffusive quantum dots.

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