SUMMARY AND OUTLOOK

Somehow I never finish what I start, I always end up ending it.
— Pushpa Rana

In this thesis, we have studied extensively the subleading term of the strongly interacting limit in Density Functional Theory, $F_{ZPE}$, with particular focus on the analytical properties and the related exact features. Such term encloses the kinetic contribution to the total correlation energy in the form of Zero Point Oscillations around the equilibrium position determined by the SCE state and could shed light on the properties of the physical system, provided a deeper understanding of its formalism is achieved.

To this end, as shown in Chapter 4, we first got confirmation that the ZPE functional might indeed be the subleading term of the SCE limit and that spin effects enter to hyper-asymptotic orders, by antisymmetrizing the ZPE wavefunction. This procedure is not trivial, as the ZPE wavefunction is typically expressed as the product of ground state harmonic oscillators orbitals in a curvilinear metric which needs to be inverted to properly introduce the fermionic statistics. While this was achieved for $N = 2$ in $d = 1$, it is still not clear how this could be generalized to higher number of particles and dimensions. Moreover, since the statistics enters in the leading term of an hyper-asymptotic series, the accuracy in computing the spin effects proved to be extremely poor, compared with the numerically accurate one. We also understood that extra care should be used in taking expectation value of operators using the ZPE wavefunction, as its inability in reproducing correctly the density to the right order in the coupling $\lambda$ hampers the comparison between quantities of relevance such as the electron-electron interaction expectation value, as discussed at the end of Chapter 3.

We then moved in Chapter 5 to calculate explicitly the functional derivative of $F_{ZPE}$, for which we made extensive use of the analytical properties of the comotion functions discussed in Chapter 3. Being the SCE limit a regime in which kinetic energy is suppressed, all the effects of kinetic correlation are not directly accessible. The ZPE formalism on the other hand, introducing explicitly the kinetic energy in $F_{ZPE}$, is naturally endowed with this capability. Using the ZPE functional derivative as an approximation to the Hartree exchange-correlation potential, we could show in a one dimensional homonuclear dimer model that $F_{ZPE}$ correctly helps building a peak in the midbond region in the regime of dissociation. Such peak however is reminiscent of the divergences of the comotion functions and as such, contrarily
to the exact result, does not saturate to the ionization energy but
diverges to $+\infty$. It would be interesting to see if this unwanted feature
could be cured by looking at the subleading terms in the Strongly
Interacting Limit expansion. To this aim, we already carried out the
explicit computation of the kinetic energy operator to the appropriate
order in $\lambda$ in appendix A. Furthermore, the functional derivative
of the ZPE functional fails to be used as an approximation to the
external potential $v^\lambda[\rho]$ since it destroys the density constraint. It is
clear that further pondering is required on how the $\lambda$-dependent
external potential which enforces the physical density at all orders
needs to be computed.

As discussed extensively in Chapters 3, 4 the ZPE functional acts
effectively as a regularization of the SCE functional. In Chapter 6,
we explored the possibility of approximate $F^{\text{ZPE}}[\rho]$ via an entropic
regularization of the SCE functional through a coupling parameter
$\tau$. It turns out that, at least for $N = 2$ and $d = 1$, an interesting
connection can be made between the minimizer of the regularized
entropic problem and the ZPE wavefunction. Since also the entropic
regularization introduces a one body potential which keeps the density
fixed to varying of $\tau$, it would be interesting to study its properties
as a function of $\tau$, in the light of gaining insights to the problems
aforementioned concerning the expansion of $v^\lambda$.

We used the concepts developed in Chapters 3, 5 to compute self-
consistently in a KS scheme the ground state densities of a one di-
ensional quantum wire at different correlation regime, testing for
the first time in the context of density functional theory a spectral
renormalization algorithm popular in non-linear optics. The algorithm
proved to be capable of handling well the SCE approximation, which
have proven to be hard to converge due to the sparsity of the problem,
as well as the ZPE approximation to Hartree and exchange correlation
potential. We also introduced a more effective way to compute the
comotion functions which does not rely on interpolations and it is
more suitable to deal with low density regimes.

The SCE limit describes a state in which particles behave as they
were a floating Wigner crystal, a remarkable phase of the electron gas
at very low density. Our interest in this system prompted us into taking
a deeper look into an apparently completely different theoretical frame,
namely a strongly interacting limit of Hartree-Fock theory. With the
analytical tools developed in the previous chapters, we tested whether
this frame could provide us with a different perspective on the Wigner
crystal and a deeper understanding of the electron gas. Within the
Einstein approximation for phonons we compute the energy of a
modified Hamiltonian, finding a value for the energy per particle in
the low density limit qualitatively comparable with other calculations.
It would be interesting to refine the computation by going beyond the
Einstein approximation, e.g. by carrying on a normal mode analysis.
Work along all these direction is in progress.
APPENDIX