RESULTADOS MATEMÁTICOS EN MECÁNICA CUÁNTICA

Multiplicidad y concentración para la ecuación de Schrödinger no-lineal con frecuencia crítica y propiedades de compacidad para operadores de traza

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Resumen de la Tesis para optar al grado de Doctor en Ciencias de la Ingeniería, Mención Modelación Matemática

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Se abordan problemas matemáticos de la Mecánica Cuántica tanto en la *representación de Schrödinger*, como en la *representación de Heisenberg*. Se presenta una breve introducción a la Teoría Cuántica.

En el marco de la representación de Schrödinger, se estudia la ecuación no-lineal de Schrödinger (E) $\varepsilon^2\Delta v - V(x)v + |v|^{p-1}v = 0$, en $\mathbb{R}^d$, y el problema límite (L) $\Delta u + |u|^{p-1}u = 0$ en Ω, $u = 0$ sobre $\partial\Omega$, donde se asume que $\Omega = \text{int}\{x \in \mathbb{R}^d : V(x) = \inf V = 0\}$ es no-vacío. Usando el esquema de Ljusternik-Schnirelman se prueba la existencia de un número infinito de soluciones para (E) y (L) que comparten la topología de sus conjuntos de nivel. Denótesen los respectivos conjuntos de soluciones por $\{v_{k,\varepsilon}\}_{k\in\mathbb{N}}$ y $\{u_k\}_{k\in\mathbb{N}}$. Se muestra que para $k \in \mathbb{N}$ fijo, módulo reescalamiento de $v_{k,\varepsilon}$, la energía de $v_{k,\varepsilon}$ converge a la energía de u_k. También se muestra que las soluciones de (E), $v_{k,\varepsilon}$, se concentran exponencialmente en torno a Ω y que, módulo reescalamiento y módulo extración de subsucesiones, tales soluciones convergen a una solución de (L).

En el marco de la representación de Heisenberg se establecen, desigualdades de interpolación tipo Gagliardo-Nirenberg. Minimizar el funcional de energía libre para un potencial dado es equivalente a probar desigualdades tipo Lieb-Thirring, en tanto que optimizar sobre el potencial produce desigualdades de interpolación. Se establecen resultados de compacidad para una clase de operadores de traza autoadjuntos que tienen energía cinética finita que son análogos a nivel de operadores de las inmersiones clásicas de Sobolev. Aplicando estos resultados a la minimización de funcionales de energía libre (no-necesariamente convexos), se caracterizan los estados estacionarios del problema de Hartree con temperatura. En la representación via estados mixtos de la Mecánica Cuántica se cumplen resultados equivalentes.

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Dedicatoria

A mis hijos, Daniel y Keren, con amor.

“Que viva en ellos el anhelo de justicia, paz y verdad.
Que superen mis buenas obras.
Que no caigan en mis equivocaciones.
Que en su descendencia siempre se hallen Justos.
Baruj HaShem!!”

Agradecimiento

Gracias al Eterno, bendito sea Su Nombre, quien sostiene la creación con Justicia, Verdad y Misericordia.

Gracias a mi esposa. Sin ella no estaría donde estoy.

Gracias a Patricio Felmer. Hombre de bien. Justo y paciente. Gran matemático. Su ayuda fue vital.

Gracias a Jean Dolbeault. Hombre de gran espíritu solidario. Gran matemático. Su ayuda fue determinante.

Il libro della natura é scrito in lingua matematica.
Galileo Galilei

Capítulo 1

Introducción General

El presente documento recopila los frutos del trabajo de investigación desarrollado durante mis estudios doctorales en Universidad de Chile y que derivó en 2 artículos científicos terminados, [35] y [27], y un artículo en su etapa final, [31]. Puesto que todos los resultados obtenidos caen en el contexto matemático de la Mecánica Cuántica, se presenta una breve introducción a dicha teoría física en el Capítulo 2.

El artículo [35] se presenta en el Capítulo 3 en Inglés tal como ha sido aceptado para su publicación. El artículo [27] se presenta en el Capítulo 4 (Secciones 4.1-4.4) tal como ha sido enviado a consideración, asimismo en Inglés. De [31] se presenta, en la Sección 4.5, el problema que motivó [27]. Cuando se ha creido menester se ha agregado detalles que por cuestión de longitud no fueron incluidos en su versión final.

1.1. Presentación

En esta tesis se abordan problemas matemáticos de la Mecánica Cuántica tanto en la *representación de Schrödinger*, como en la *representación de Heisenberg*. Sucintamente presentamos en las Secciones 1.1.1 y 1.1.2 respectivamente los resultados más importantes de los trabajos [35] y [27] que aparecen en los Capítulos 3 y 4.

1.1.1. Multiplicidad y concentración para la ecuación de Schrödinger no-lineal con frecuencia crítica

La ecuación no-lineal de Schrödinger aparece frecuentemente en muchos campos de la física[1] y toma usualmente la forma

$$i\hbar\Psi_t + \frac{\hbar^2}{2}\Delta\Psi - V_o(x)\Psi + |\Psi|^{p-1}\Psi = 0, \quad \forall x \in \mathbb{R}^d, \forall t \geq 0, \tag{1.1}$$

donde $p > 1$ y $\hbar$ denota la constante de Plank. En el Capítulo 3 abordamos el estudio de existencia y propiedades cualitativas de ondas estacionarias que verifican (1.1), esto es, soluciones que tienen la forma

$$\Psi(x,t) = v(x) \cdot e^{-iEt/\hbar}.$$

De manera especial nos interesa el comportamiento de las soluciones cuando $\hbar$ tiende a cero, es decir el límite semi-clásico.[2] En términos de $v = v(x)$, el problema puede ser escrito como

$$\begin{cases} \varepsilon^2\Delta v - V(x)v + |v|^{p-1}v = 0, & \text{in} \quad \mathbb{R}^d; \\ \qquad v(x) \to 0, & \text{as} \quad |x| \longrightarrow \infty \end{cases}, \tag{P_ε}$$

donde

$$\begin{cases} \varepsilon^2 = \hbar^2/2, \\ V(x) = V_0(x) - E, \quad x \in \Omega. \end{cases}$$

Aquí suponemos que $d \geq 3$ y $1 + p \in (2, 2^*)$, con $2^* = \frac{2d}{d-2}$.

Ha habido un gran número de trabajos de investigación para el caso en que el potencial V es positivo. Esta concurrencia tuvo su génesis en el trabajo de Floer y Weinstein [37], donde se muestra que en el caso unidimensional, para $p = 3$, hay una familia de soluciones que se concentran entorno a un punto crítico no-degenerado del potencial. Estas soluciones, v_ε, son capturadas usando un método de reducción de Lyapunov-Schmidt y satisfacen

$$\liminf_{\varepsilon\to 0} \max_{x\in\mathbb{R}^d} |v_\varepsilon(x)| > 0. \tag{1.2}$$

Otros trabajos fueron llevados a cabo por varios autores: Oh [61], Wang [75], Rabinowitz [63], del Pino y Felmer [22], [23], Ambrosetti et al. [1], Gui [43], Li [54], Dancer y Yan [16], Kang y Wei [50] y otros.

[1] Véase el Ejemplo 2.5.
[2] Véase la Sección 2.4

En tales trabajos, las soluciones encontradas verifican (1.2) y se concentran en ciertos puntos críticos del potencial y decaen exponencialmente conforme uno se aleja de ellos. En estos trabajos se usan diferentes herramientas, basadas ya sea en el método variacional o en la reducción de Lyapunov-Schmidt, o en una combinación de estos. En estos caso, las propiedades de las soluciones positivas de la ecuación límite son usadas extensivamente para obtener los resultados. En particular, bajo la metodología de Lyapunov-Schmidt, se usa el hecho de que la única solución positiva de la ecuación límite es no-degenerada.

En contraste con el caso de un potencial positivo, hay un par de trabajos recientes de Byeon y Wang [11, 12], donde se considera un potencial no-negativo cuyo conjunto de ceros $\Omega \subset \mathbb{R}^d$ está acotado. El primer hecho importante es que para las soluciones encontradas en [11] y [12], (1.2) deja de ser válido; de hecho, el valor máximo de las soluciones tiende a cero, con una rapidez que depende tanto de la naturaleza del conjunto Ω como de la estructura de la ecuación límite que le corresponda. Los autores distinguen tres casos:

1. $\Omega = \operatorname{int} \overline{\Omega} \neq \emptyset$, que es referido como el *flat case*,
2. $\overline{\Omega}$ es un conjunto finito de puntos, y V se acerca a cero polinomialmente en $\overline{\Omega}$, que es referido como el *finite case*, y
3. $\overline{\Omega}$ es un conjunto finito de puntos, y V se acerca a cero exponencialmente, que es referido como el *infinite case*.

Nosotros consideramos el flat case, es decir, cuando el interior del conjunto de ceros de V, $\overline{\Omega}$, es un conjunto acotado no vacío. En este contexto la ecuación límite es

$$\begin{cases} \Delta u + |u|^{p-1}u = 0, & \text{in} \quad \Omega; \\ \qquad u = 0, & \text{on} \quad \partial\Omega \end{cases} \tag{P}$$

Byeon y Wang probaron en [11] que soluciones de mínima energía de (P_ε) convergen, via un reescalamiento apropiado, a soluciones de mínima energía de (P). Más aún, muestran que soluciones de mínima energía de (P_ε) se concentran en Ω; esto, al probar su decaimiento exponencial fuera de Ω. En el caso en que Ω tiene varias componentes conexas, los autores pueden determinar en qué componente tendrá lugar la concentración.

Si analizamos con mayor cuidado el problema límite (P) nos damos cuenta que a la par de las soluciones de mínima energía hay muchas más soluciones. En particular, la aplicación de la teoría de Ljusternik-Schnirelman para funciones pares provée la existencia de un número infinito de soluciones. Es entonces natural preguntarse si el problema (P_ε) tiene un número infinito de soluciones y cuál es su relación con las soluciones de (P). En el Capítulo 3 damos respuesta a esta pregunta cuando Ω es conexo. Probamos que (P_ε) tiene infinitas soluciones tipo Ljusternik-Schnirelman cuyos niveles críticos convergen a los niveles críticos de (P). Más aún, probamos que estas soluciones también se concentran en Ω.

Ahora presentamos nuestros resultados. Suponemos que el potencial $V(x)$ verifica:

(V1) V es una función continua no-negativa sobre $\mathbb{R}^d$.

(V2) $V(x) \to \infty$ cuando $|x| \to \infty$.

(V3) $\Omega = \mathrm{int}\{x \in \mathbb{R}^d \,|\, V(x) = 0\} \neq \emptyset$ es conexo y con frontera suave.

Consideramos el funcional

$$J_\varepsilon(w) = \frac{1}{2}\int_{\mathbb{R}^d}\left(|\nabla w|^2 + \frac{1}{\varepsilon^2}V(x)w^2\right)dx, \tag{1.3}$$

definido sobre

$$\mathcal{M}_\varepsilon = \{w \in H_\varepsilon :\; ||w||_{L^{p+1}(\mathbb{R}^d)} = 1\},$$

donde

$$H_\varepsilon \equiv \left\{ w \in \mathrm{H}^1(\Omega) :\; ||w||_\varepsilon \equiv \left(\int_{\mathbb{R}^N} |\nabla w|^2 + \frac{V(x)}{\varepsilon^2}w^2\right)^{1/2} < \infty \right\}.$$

Los puntos críticos de J_ε sobre $\mathcal{M}_\varepsilon$ dan lugar, via reescalamiento, a las soluciones de (P_ε). En nuestro contexto, la ecuación lí mite para (P_ε) es (P). Asociado a (P) consideramos el funcional

$$J(u) = \frac{1}{2}\int_\Omega |\nabla u|^2 dx, \tag{1.4}$$

definido sobre

$$\mathcal{M} = \{u \in \mathrm{H}^1_0(\Omega) :\; ||u||_{L^{p+1}(\Omega)} = 1\}.$$

Los puntos críticos de J sobre $\mathcal{M}$ son, via reescalamiento, las soluciones de (P). Nuestro resultado principal es:

Teorema 1.1. *Bajo nuestras hipótesis generales (V1), (V2) y (V3) sobre el potencial, y suponiendo que $d \geq 3$ y $1 < p < (d+2)/(d-2)$, tenemos:*

i) *Dado $\varepsilon > 0$, el funcional J_ε posée infinitos puntos críticos $\{\hat{w}_{k,\varepsilon}\}_{k\in\mathbb{N}} \subset \mathcal{M}_\varepsilon$.*

ii) *El funcional límite J tiene infinitos puntos críticos $\{\hat{w}_k\}_{k\in\mathbb{N}} \subset \mathcal{M}$.*

iii) *Dado $k \in \mathbb{N}$, los valores críticos satisfacen*

$$\lim_{\varepsilon\to 0} J_\varepsilon(\hat{w}_{k,\varepsilon}) = J(\hat{w}_k). \tag{1.5}$$

iv) *Más aún, dado $\delta, c > 0$, existe un $\varepsilon_0 > 0$ tal que*

$$|\hat{w}_{k,\varepsilon}(x)| < C \cdot \exp\{-\frac{c}{\varepsilon} \cdot \operatorname{dist}(x, \Omega^\delta)\}, \quad \forall x \in \mathbb{R}^d, \forall \varepsilon \in]0, \varepsilon_0), \tag{1.6}$$

donde $C > 0$ y $\Omega^\delta = \{x \in \mathbb{R}^d : \operatorname{dist}(x, \Omega) < \delta\}$.

v) *Sobre la frontera de Ω, las funciones $\hat{w}_{k,\varepsilon}$ verifican*

$$\lim_{\varepsilon\to 0} \max_{x\in\partial\Omega} |\hat{w}_{k,\varepsilon}(x)| = 0, \quad \forall k \in \mathbb{N}. \tag{1.7}$$

Es claro que las funciones

$$v_{k,\varepsilon} = (2\varepsilon^2 c_{k,\varepsilon})^{1/(p-1)}\hat{w}_{k,\varepsilon}, \qquad c_{k,\varepsilon} = J_\varepsilon(\hat{w}_{k,\varepsilon})$$

son soluciones de (P_ε) y, como corolario, satisfacen, para $k \in \mathbb{N}$ fijo,

$$\lim_{\varepsilon\to 0} ||v_{k,\varepsilon}||_{L^\infty(\mathbb{R}^d)} = 0 \tag{1.8}$$

y

$$\liminf_{\varepsilon\to 0} \frac{||v_{k,\varepsilon}||_{L^\infty(\mathbb{R}^d)}}{\varepsilon^{2/(p-1)}} > 0. \tag{1.9}$$

No es difícil ver que las funciones $w_{k,\varepsilon} = (2c_{k,\varepsilon})^{1/(p-1)}\hat{w}_{k,\varepsilon}$ satisfacen la ecuación

$$\begin{cases} \Delta w - \varepsilon^{-2}V(x)w + |w|^{p-1}w = 0, & \text{in} \quad \mathbb{R}^d; \\ w(x) \to 0, & \text{as} \quad |x| \longrightarrow \infty \end{cases} \tag{P'_ε}$$

Para cada k, probamos la existencia de una subsucesión de $w_{k,\varepsilon}$ que converge a w_k, una solución de (P).

El comportamiento descrito por nuestra sucesión de soluciones corresponde al mismo fenómeno discutido por Byeon y Wang, ([11, Th.2.2]), para soluciones de mínima energía positivas. La propiedad (1.8) contrasta al comportamioento en el caso no-crítico, $\text{ínf}_{x\in\mathbb{R}^d} V(x) > 0$, donde todas las soluciones de (P_ε) mantienen sus máximos estrictamente por encima de cero.

En [11] se muestra que el reescalamiento $w_\varepsilon = \varepsilon^{-2/(p-1)} v_\varepsilon$ sub-converge[3] puntualmente a una solución de mínima energía U de (P), en Ω, y a 0 en $\mathbb{R}^d \setminus \Omega$. Más aún, dado $\delta > 0$, la convergencia es uniforme sobre $\{x \in \mathbb{R}^d : \text{dist}(x, \partial\Omega) \geq \delta\}$.

El potencial que nosotros consideramos es no-negativo y se hace cero en un conjunto abierto Ω. Esta situación se considera crítica pues, en el límite, el comportamiento de las soluciones es muy diferente. Para el caso de un potencial-positivo, las soluciones de mínima energía deben concentrarse necesariamente en un punto; sin embargo, para un potencial que alcanza el cero la concentración ocurre en todo el conjunto Ω. Cuando el potencial se vuelve negativo en un conjunto acotado, ya no tiene sentido hablar de soluciones de mínima energía. Sin embargo, esta situación puede todavía ser bien entendida, al menos en el caso unidimensional y en el caso radial, como en los trabajos [36, 15].

No decimos nada respecto al signo de las soluciones encontradas; sin embargo, puesto que el problema límite (P) pudiera tener muchas soluciones positivas dependiendo de la geometía de Ω (véase e.g. [17]), lo mismo podría suceder con (P_ε).

En nuestro trabajo consideramos sólo el caso de un potencial que diverge a infinito cuando $|x| \to \infty$, es decir verificando (V2), y desvaneciéndose en un conjunto abierto, conexo y con frontera suave, es decir verificando (V3). Pensamos que nuestros resultados siguen siendo válidos para potenciales más generales, cuando el conjunto de ceros de V no es conexo, y también para los caso finito e infinito. Particularmente interesante es el caso de un potencial acotado, positivo al infinito. En este caso la existencia de infinitos puntos críticos como en el Teorema 1.1, i) podría dejar de ser válido. Sin embargo, los puntos ii)-v), con k fija, deberían ser válidos.

[3]Se dice que una familia de funciones $\{f_\varepsilon\}_{\varepsilon>0}$ sub-converge en un espacio X, mientras $\varepsilon \to 0$, cuando de cualquier sucesión $\{\varepsilon_i\}_{i\in\mathbb{N}}$ convergente a cero, es posible extraer una subsucesión $\{\varepsilon_{n_i}\}_{i\in\mathbb{N}}$ tal que $\{f_{\varepsilon_{n_i}}\}_{i\in\mathbb{N}}$ converge en X, cuando $i \to \infty$.

De hecho, después que concluimos nuestro estudio, conocimos de un trabajo reciente de Ding y Szulkin [24] donde este problema es tratado. En lugar de las condiciones (V2) y (V3) los autores suponen que

(V2') existe $b > 0$ tal que el conjunto $\{x \in \mathbb{R}^d : V(x) < b\}$ es no-vacío y tiene medida finita.

Fijando $k \in \mathbb{N}$, prueban que para algún $\Lambda_k > 0$, el problema (P_ε) tiene al menos k pares de soluciones en H_ε cuando $\varepsilon \in]0, \Lambda_k^{-1/2}[$. En contraste, nosotros probamos la existencia de un número infinito de soluciones, al menos un par para cada nivel de energía. Muestran que si para cada $m \in \mathbb{N}$, u_m es una solución de (P_{ε_m}), donde $\lim_{m\to\infty} \varepsilon_m = 0$, entonces u_m converge en H_1 a alguna solución u de (P) suponiendo el acotamiento de $(||u_m||_{\varepsilon_m})_{m\in\mathbb{N}}$. Nosotros probamos esta última condición para cada nivel k de energía. Probamos asimismo que nuestras soluciones $(w_{k,\varepsilon})$ subconvergen en $\mathrm{H}^1(\Omega)$ a alguna solución de (P).

Finalmente señalemos que en nuestro trabajo no sólo obtenemos el decaimiento exponencial de las soluciones al infinito sino que, adicionalmente, obtenemos estimaciones asintóticas sobre el comportamiento en la frontera del dominio.

1.1.2. Propiedades de compacidad para operadores de traza

El primer valor propio $\lambda_{V,1}$ de un operador de Schrödinger $-\Delta + V$ puede ser estimado usando desigualdades de Sobolev, [72, 68, 42]. En artículos recientes, [7, 73, 26], una conexión precisa ha sido establecida entre las estimaciones optimales de $\lambda_{V,1}$ en términos de una norma de V y las constantes optimales de algunas desigualdades tipo Gagliardo-Nirenberg, [76, 26].

En el caso de sistemas ortonormales y sub-ortonormales, desigualdades de interpolación tipo Gagliardo-Nirenberg provéen información sobre las constantes optimales[4] en desigualdades que pueden ser extendidas a desigualdades tipo Lieb-Thirring, [55]. En [26] se pueden hallar referencias en esta dirección y proposiciones precisas respecto de la relación entre constantes optimales para estas dos familias de desigualdades, en el caso del espacio euclideano $\mathbb{R}^d$.

[4]Véase [57, 56, 40, 32].

Inversamente, el conocimiento de desigualdades de Lieb-Thirring puede ser replanteado en términos de desigualdades de interpolación para *estados mixtos* que son sistemas infinitos de funciones ortogonales con números de ocupación, véase [26]. Se sabe que una formulación equivalente es válida en términos de operadores. En este trabajo reescribimos y extendemos estas desigualdades de interpolación para *operadores de traza autoadjuntos* y nos centramos en el caso de un dominio $\Omega \subset \mathbb{R}^d$. También estudiamos, a nivel de operadores, las *propiedades de compacidad* de las correspondientes inclusiones, que extienden las propiedades bien conocidas de las inmersiones de Sobolev.

De gran motivación es el artículo de P. Markowich, G. Rein y G. Wolansky, [60], que fue dedicado al análisis de la estabilidad del sistema de Schrödinger-Poisson. Allí participan de manera crucial algunos funcionales que son clave para nuestro planteo y que llamaremos *funcionales de energía libre* debido a su interpretación en física. En [60], los autores se refieren a tales funcionales como funcionales de *Casimir* por razones históricas en mecánica, [77]. Recientemente, varios resultados basados en funcionales de energía libre, que a veces son también llamados *funcionales de entropía generalizada*, han sido obtenidos en la teoría de ecuaciones en derivadas parciales. Podemos señalar, por ejemplo, resultados de estabilidad no-lineal para ecuaciones cinéticas y de fluidos, véase [77, 44, 45, 67], estudios sobre el comportamiento cualitativo de las soluciones de ecuaciones cinéticas y de difusión incluyendo límites de difusión, véase e.g. [6, 14, 29], y aplicaciones a problemas de frontera libre: [30], o mecánica cuántica: [59, 60]. A nivel formal esta variedad de funcionales corresponden a un mismo objeto. La conexión precisa está todavía siendo estudiada desde un punto de vista matemático, si bien la correspondencia a nivel físico no deja dudas.

Minimizar el funcional de energía libre para un potencial dado es equivalente a probar desigualdades de Lieb-Thirring, en tanto que la optimización sobre el potencial provée desigualdades de interpolación. Tales puntos han sido estudiados apenas tangencialmente en [60], pues en este artículo el potencial es dado por una ley electrostática de Poisson con condición de Dirichlet homogénea sobre la frontera, así que es siempre positivo. Nosotros trabajamos en un contexto mucho más general que físicamente podría corresponder a potenciales externos con una singularidad y nuestra primera tarea es, por tanto, acotar por debajo al funcional de energía libre, *i.e.* establecer versiones adaptadas de las desigualdades de Lieb-Thirring. Nuestro segundo paso consiste en reformular estas desigualdades en términos de desigualdades tipo Gagliardo-Nirenberg para operadores, y estudiar las propiedades de compacidad de las correspondientes inmersiones. En estas instancias, el proceso de minimización se vuelve más o menos trivial, proveyendo casi gratuitamente la existencia de minimizadores, incluso para el caso de modelos no-lineales por ejemplo con un acoplamiento de Poissson.

Sea $\Omega \subset \mathbb{R}^d$ un dominio con frontera suave y consideremos un potencial suave y positivo V sobre $\overline{\Omega}$. Para empezar, estamos interesados en desigualdades tipo Lieb-Thirring para el operador de Schrödinger $-\Delta + V$. Sea $\{\lambda_{V,i}\}_{i\in\mathbb{N}}$ la correspondiente sucesión no-decreciente de valores propios. Como una directa consecuencia de los resultados de [26], la siguiente desigualdad se cumple: para todo $\gamma > d/2$, existe una constante explícita $C(\gamma)$, que no depende de V, tal que

$$\sum_{i\in\mathbb{N}} \big(\lambda_{V,i}\big)^{-\gamma} \leq C(\gamma) \int_\Omega V^{d/2-\gamma}\, dx \,, \tag{1.10}$$

(véase el Ejemplo 1 en la Sección 4.3.1 para un enunciado preciso). Esta desigualdad resulta en un caso especial de una desigualdad *maestra* que en seguida introducimos. Considérese una sucesión de funciones ortonormales $\{\psi_i\}_{i\in\mathbb{N}}$ y una sucesión $\{\nu_i\}_{i\in\mathbb{N}}$ de reales no-negativos. A la sucesión $\{(\nu_i,\psi_i)\}_{i\in\mathbb{N}} \in \ell^1 \times \mathrm{L}^2(\Omega)$ se le conoce en física como un *estado mixto*. La *desigualdad maestra* es

$$\begin{aligned} \sum_{i\in\mathbb{N}} \beta(\nu_i) + \frac{1}{2}\sum_{i\in\mathbb{N}} \nu_i \big(\psi_i, (-\Delta + V)\,\psi_i\big)_{L^2(\Omega)} &\geq -\sum_{i\in\mathbb{N}} F\big(\lambda_{V,i}\big) \\ &\geq -\int_\Omega G(V)\, dx \,. \end{aligned} \tag{1.11}$$

Entonces (1.10) corresponde al caso $\beta_m(\nu) = -c_m\,\nu^m$ para una constante explícita c_m, $m = \gamma/(\gamma+1) \in (d/(d+2), 1)$, $F(s) \equiv s^{-\gamma}$ y $G(s) \equiv C(\gamma)\, s^{d/2-\gamma}$. El hecho importante es que la desigualdad (1.11) entonces se verifica para todo potencial y todo estado mixto. Se puede hacer otras elecciones, por ejemplo $\beta_1(s) \equiv s\log s - s$, $F(s) \equiv e^{-s}$ y $G(s) \equiv (4\pi)^{-d/2}\, e^{-s}$, que provée entonces la siguiente desigualdad tipo Lieb-Thirring

$$\sum_{i\in\mathbb{N}} e^{-\lambda_{V,i}} \leq (4\pi)^{-d/2} \int_\Omega e^{-V}\, dx \,.$$

Usando el teorema de Hilbert-Schmidt, al considerar operadores de traza autoadjuntos L con kernel $K_L(x,y) \equiv \sum_{i\in\mathbb{N}} \nu_i\, \psi_i(x)\, \psi_i(y)$, podemos reformular la primera parte de la desigualdad (4.2) en términos de operadores y así obtener

$$\mathrm{Tr}\,[\beta(L) + (-\Delta + V - \lambda)\, L] \geq -\mathrm{Tr}\,\big[F\big(-\Delta + V - \lambda\big)\big]$$

para algún parámetro λ que por el momento lo tomamos igual a 0. Hasta ahora, V se supuso positiva. Nuestro primer resultado importante es una extensión de la desigualdad (1.11) a potenciales que podrían cambiar de signo. Para una perturbación W de un potencial V que cambia de signo, la desigualdad (4.2) es reemplazada por

$$\mathrm{Tr}\,[\beta(L) + (-\Delta + V + W - \lambda)\, L] \geq -\,\varepsilon^{-d/2} \int_\Omega G(W)\, dx\,, \qquad (1.12)$$

para ciertos valores ε y λ a ser fijados posteriormente. Una optimización en W entonces provée una desigualdad de interpolación tipo Gagliardo-Nirenberg. Para un enunciado preciso, fijemos algo de notación. Consideramos una función no-negativa f verificando $\int_0^\infty f(t)\, \big(1 + t^{-d/2}\big)\, t^{-1}\, dt < \infty$. Ponemos

$$F(s) := \int_0^\infty e^{-t\,s}\, f(t)\, \frac{dt}{t} \quad \text{y} \quad G(s) := \int_0^\infty e^{-t\,s}\, (4\pi\, t)^{-d/2}\, f(t)\, \frac{dt}{t}\,.$$

Sean β y τ tales que $\beta(s) \equiv F^*(-s)$ y $G(s) \equiv \tau^*(-s)$. Aquí F^* denota la transformada de Legendre-Fenchel de F. También usamos la notación ρ_L para la función no-negativa $\sum_{i\in\mathbb{N}} \nu_i\, |\psi_i|^2 \in L^1(\Omega)$, usando una representación en estados mixtos $\{(\nu_i, \psi_i)\}_{i\in\mathbb{N}}$ asociada a L. Algunas consideraciones estándar son necesarias para identificar $\rho_L(x)$ con $K_L(x,x)$.

Teorema 1.2. *Para un potencial V, supóngase que para algún $\varepsilon \in (0,1)$, el operador $-(1-\varepsilon)\,\Delta + V$ está acotado inferiormente por alguna constante λ. Con las anteriores notaciones, la desigualdad (1.12) se verifica para cualquier operador de traza L no-negativo y autoadjunto y, más aún,*

$$\mathrm{Tr}\,[\beta(L) + (-\Delta + V - \lambda)L] \geq \varepsilon^{-\frac{d}{2}} \int_\Omega \tau\left(\varepsilon^{\frac{d}{2}}\, \rho_L(x)\right)\, dx\,.$$

El núcleo de la demostración yace en una minimización con respecto al estado mixto $\{(\nu_i, \psi_i)\}_{i\in\mathbb{N}}$, que al final requiere que ψ_i sea una función propia de $-\Delta + V$ y $\nu_i = (\beta')^{-1}(\lambda - \lambda_{V,i})$. Puesto que el dominio Ω está acotado, al menos cuando $V \equiv 0$ y $\lambda = 0$, estas desigualdades pueden ser ligeramente mejoradas, pero la mejora en la constante depende de Ω; la desigualdad anterior así como la desigualdad (1.12) son óptimos si uno busca constantes que sean independientes de Ω.

En los interesantes casos $F(s) \equiv s^{-\gamma}$ y $F(s) \equiv e^{-s}$, obtenemos las siguientes desigualdades de interpolación

$$\mathrm{Tr}\,[-\Delta L] + \kappa(\gamma) \int_\Omega \rho_L^q \, dx \geq c_m \, \mathrm{Tr}\,[L^m] \ ,$$

donde $q \equiv (2\gamma - d)/(2(\gamma+1) - d) \in (0,1)$ y $\kappa(\gamma)$ es una constante positiva explícita, y

$$\int_\Omega \rho_L \log \rho_L \, dx \leq \mathrm{Tr}\,[L \, \log L] + \frac{d}{2} \log \left(\frac{e}{2\pi d} \, \frac{\mathrm{Tr}\,[-\Delta L]}{\|L\|_1} \right) \|L\|_1 \ ,$$

donde L es cualquier operador de traza no-negativo y autoadjunto. Para no complicar las cosas, las desigualdades aquí escritas corresponden al caso en que V es no-negativa, pero enunciados más generales respecto a potenciales que cambian de signo pueden ser deducidos a partir del Teorema 1.2. Véase el Teorema 4.3 y los Corolarios 4.1, 4.3, 4.4, 4.5 para varias mejoras.

Las desigualdades de interpolación del Teorema 1.2 generalizan para operadores de traza autoadjuntos las desigualdades de Gagliardo-Nirenberg usuales. Así como para la inmersión $\mathrm{H}^1_0(\Omega) \hookrightarrow \mathrm{L}^2(\Omega)$, alguna compacidad se puede avisorar. Tal enunciado constituye nuestro segundo resultado.

Teorema 1.3. *Bajo las hipótesis del Teorema 1.2, si $\{L_n\}_{n\in\mathbb{N}^*}$ es una sucesión de operadores autoadjuntos no-negativos con traza acotada tal que*

$$\{\mathrm{Tr}\,[\beta(L_n) + (-\Delta + V - \lambda)\, L_n]\}_{n\in\mathbb{N}^*}$$

está también acotada, entonces $\{L_n\}_{n\in\mathbb{N}^*}$ es relativamente compacta y converge (módulo subsucesiones) a algún operador compacto autoadjunto no-negativo L. Más aún, ρ_{L_n} converge a ρ_L in $L^q(\Omega)$, para todo $q \in [1,\infty]$ si $d=1$, $q \in [1,\infty)$ si $d=2$ y $q \in [1, d/(d-2)]$ si $d \geq 3$.

En el Capítulo 4 empezamos introduciendo definiciones, resultados preliminares y consecuencias de los resultados de [26]. Luego presentamos un conjunto de operadores de traza que tienen la forma $F(-\Delta)$. A esta clase se pertenecen los operadores generados por la distribución de Boltzmann y la estadística de Fermi-Dirac. El espacio $\mathcal{S}_1$ de *operadores de traza autoadjuntos*, también conocidos como *operadores nucleares autoadjuntos*, juega el rol del espacio L^1 y los espacios $\mathcal{S}_q$ se pueden percibir como los espacios L^q, $q \in [1, \infty]$. Inspirados por esta analogía, definimos los conos tipo Sobolev $\mathcal{W}^{l,p}$ como subconjuntos apropiados de $\mathcal{S}_1$. Hasta donde sabemos la definición de estos conos es una novedad. Probamos entonces propiedades básicas de estos conos y un resultado de regularidad sobre las funciones de densidad asociadas a $\mathcal{H}^1 = \mathcal{W}^{1,2}$. Luego definimos el *funcional de energía libre*

$$\mathcal{F}^{\lambda}_{V,\beta}(L) \equiv \mathrm{Tr}\left[\beta(L) + (-\Delta + V - \lambda)L\right].$$

Los Teoremas 1.2 y 1.3 y una desigualdad de interpolación mejorada se prueban a continuación. La estimación clave es una desigualdad convexa que permite simultáneamente minimizar el *funcional de energía libre* y conseguir alguna coercitividad aun si V cambia de signo. Sigue entonces el resultado de compacidad y, como una consecuencia simple, probamos la existencia de minimizadores en varios casos de interés en Mecánica Cuántica.

1.2. Reconocimiento

Quiero reconocer a todos los estamentos de Universidad de Chile que de una u otra manera apoyaron mi proyecto doctoral. En especial y sobremanera, presento mi más sincero sentimiento de gratitud al Prof. Patricio Felmer quien con importantes consejos y críticas constructivas ha permitido que este trabajo tenga la calidad con que se presenta.

Una buena parte de mi investigación la desarrollé en el Centre De Recherche en Mathématiques de la Décision - Université Paris Dauphine. Allí conté con todas las facilidades y gocé de una remarcable hospitalidad. Quiero agradecer al Prof. Jean Dolbeault quien supervisó generosamente mi trabajo durante mi estancia en Francia.

Finalmente quiero hacer público mi agradecimiento al Gobierno de Chile que a través de una beca del Proyecto MECESUP UCH0009 financió mis estudios doctorales. Mi estadía en Francia fue financiada parcialmente por los Proyectos ECOS-Conicyt # C02E08 y # C05E09 y por el programa europeo Alfa.

1.3. Convenciones

Mencionemos las principales convenciones que guardamos a lo largo del documento.

Dados dos conjuntos $X \subset Y$, denotaremos por Id la función de inclusión; si $X = Y$, Id es la identidad. Si f y g son dos funciones sobre un conjunto no-vacío A, su compuesta será denotada por $f \circ g$.[5] Si $(A, +)$ constituye un grupo, el conmutador de f y g está dado por $[f, g] = f \circ g - g \circ f$.

Por $\mathbb{N}$, $\mathbb{R}$ y $\mathbb{C}$ denotaremos respectivamente los conjuntos de los números naturales, reales y complejos. Por $\{x_i\}_{i\in\mathbb{N}} \subset A$ denotaremos una sucesión en un conjunto no vacío A. Dados $j, k \in \mathbb{N}$, δ_{jk} denota el delta de Kronecker, esto es $\delta_{jk} = 1$ si $j = k$ y $\delta_{jk} = 0$ en caso contrario.

El espacio euclídeo de dimensión $d \in \mathbb{N}$ será notado $\mathbb{R}^d$. Salvo que se especifique, consideraremos que la dimensión es general: $d \in \mathbb{N}$. Decimos que $\Omega \subset \mathbb{R}^d$ es un dominio si es abierto y conexo.

Dado $z = a + ib \in \mathbb{C}$, ponemos $\mathrm{Re}\, z = a$, $\mathrm{Im}\, z = b$ y $\bar{z} = a - bi$. Para las normas en $\mathbb{R}^d$ y $\mathbb{C}$ usaremos $|\cdot|$. Dados $m, n \in \mathbb{N}$, el espacio de matrices $m \times n$ sobre un campo K será denotado $M_{mn}(K)$. La matriz identidad de dimención d será denotada I^d.

Las partes positiva y negativa de $x \in \mathbb{R}$ están definidas respectivamente por $x_+ = \max(x, 0)$ y $x_- = \max(-x, 0)$, así que $|x| = x_+ + x_-$.

Dado un espacio de medida (X, μ) y $p \in [1, \infty[$, escribiremos

$$\mathrm{L}^p(X) = \left\{ f : X \longrightarrow \mathbb{C} : \ ||f||_{L^p(X)} = \left(\int_X |f|^p d\mu \right)^{1/p} < \infty \right\}$$

y pondremos $\mathrm{L}^\infty(X) = \{f : X \longrightarrow \mathbb{C} : \ ||f||_{L^\infty(X)} = \text{ess sup } |f| < \infty\}$. Para el producto escalar de $\mathrm{L}^2(X)$ usaremos la notación

$$(f,\, g)_{\mathrm{L}^2(X)} = \int_X \bar{f}\, g\, d\mu.$$

Todas las integrales sobre dominios en $X = \mathbb{R}^d$, se entenderán en el sentido de Lebesgue.

[5] En donde no se especifique se deberá asumir que las operaciones indicadas se pueden realizar.

Dado un espacio topológico X, por $\overline{A}$ entenderemos la clausura o adherencia de $A \subset X$. Si $\mathrm{dist}(\cdot,\cdot)$ es una métrica sobre X, la bola con centro en $x \in X$ y radio $r > 0$ será representada por $B(x,r)$. Si f y g son dos funciones de X en $\mathbb{R}$, la notación $f = o(g)$ quiere decir que $f/g \longrightarrow 0$ (en un régimen asintótico que será claro en su contexto); por $f = O(g)$ entendemos que f/g está acotada.

Dados X e Y, espacios topológicos, notaremos con $\mathrm{C}(X;Y)$ al espacio de las funciones continuas de X en Y y ponemos $\mathrm{C}_0(X;Y) = \{f \in \mathrm{C}(X;Y) : \mathrm{supp}(f) \text{ es compacto}\}$. En particular, si $Y = \mathbb{R}$, notaremos $\mathrm{C}(X) = \mathrm{C}(X;\mathbb{R})$. Si X e Y son variedades o espacios de Banach, $\mathrm{C}^k(X;Y)$ denotará el espacio de funciones continuamente diferenciables hasta el orden $k \in \mathbb{N}$.

Notaremos por ∇ al operador nabla, esto es,

$$\nabla = (\partial_1, ..., \partial_d)\,,$$

donde para $i \in \{1,...,d\}$, ∂_i representa la derivación parcial con respecto a la variable x_i. El gradiente de un campo escalar V y la divergencia de un campo vectorial W son $\mathrm{grad}(V) = \nabla V$ y $\mathrm{div}(W) = \nabla \cdot W$ respectivamente. El laplaciano de V se notará $\Delta V = \nabla \cdot \nabla V$.

Para la numeración de teoremas, lemas, etc. se ha tomado como referencia capítulos; por ejemplo, al hablar de la Definición 2.1 nos referimos a la primera definición que aparece en el capítulo 2. El símbolo □ indica el fin de una demostración. En lo posible, la notación y terminología utilizadas son las más usadas en el ambiente matemático. Para recalcar, cuando se introduce por primera vez un concepto X, aparecerá normalmente como concepto X y, en circunstancias especiales aparecerá como **concepto X**.

Hemos usado como referencias “base” las siguientes:

- Teoría de la Medida y Probabilidades: [3, 8, 47]
- Análisis: [9, 64, 51, 52, 34];
- Teoría de Operadores: [64, 65, 66];
- Ecuaciones Diferenciales Parciales: [33, 41, 9, 48];
- Análisis Variacional/ no-Lineal: [71, 69, 62];
- Mecánica Cuántica: [53, 46, 18];

Capítulo 2

Una introducción a la Mecánica Cuántica

Presentamos en este capítulo, una introducción breve al marco de la Mecánica Cuántica. Hemos usado como principales referencias [46] y [53].

2.1. Origen de la Mecánica Cuántica

La Teoría Cuántica nace de la imposibilidad de explicar el espectro de radiación de los cuerpos negros por medio de la electrodinámica clásica. Un cuerpo negro consiste en una cavidad cerrada mantenida a una temperatura uniforme T. Las paredes de esta cavidad emiten y absorven las radiaciones electromagnéticas que entran por un pequeño hoyo y contribuyen de esta manera a mantener el interior de la cavidad como un sistema de radiaciones electromagnéticas en equilibrio termodinámico a la temperatura T. Ahora bien, si denotamos por ν la frecuencia de la radiación y por $U(\nu)d\nu$ la cantidad de energía en la gama de frecuencias $[\nu, \nu + d\nu]$, tenemos por un lado, a partir de la experiencia, que

$$U(\nu) \approx \nu^3 \exp\left(-\frac{h\nu}{k_B T}\right), \tag{2.1}$$

donde k_B es una constante universal[1] y h es una constante determinada empíricamente. Por otro parte, la electrodinámica clásica conduce a la Ley

[1] La constante de Boltzmann, k_B, corresponde a $k_B \approx 1{,}3806503 \times 10^{-23}\ J/K$.

de Rayleigh-Jeans:

$$U(\nu) = k_B T \nu^2. \tag{2.2}$$

Conforme a (2.2), la energía electromagnética total sería $\int_0^\infty U(\nu)d\nu = \infty$ lo que no es cierto. En todo caso, obsérvese que (2.1) y (2.2) coinciden para frecuencias bajas ν.

Para levantar esta divergencia entre el modelo clásico y la experiencia, Planck formuló la siguiente hipótesis, conocida como el Principio de cuantificación de la energía de los osciladores, "*La energía de una radiación de frecuencias ν no puede tomar todos los valores posibles sino, solamente, múltiplos enteros de la energía fundamental $h\nu$, donde h es una constante universal*". En otras palabras, la energía de una radiación luminosa está "*cuantificada*". Al paquete de energía fundamental $h\nu$ se le llama "*cuanto* de energía".

2.2. Principios de la Mecánica Cuántica

Cuando se trata de aplicar la Mecánica y Electrodinámica Clásicas al nivel atómico, se presentan fuertes discordancias con los resultados experimentales. Considérese, por ejemplo, un átomo donde los electrones giran alrededor del núcleo siguiendo órbitas clásicas. Puesto que en todo movimiento acelerado de cargas hay una emisión continua de ondas electromagnéticas, cada electrón debería perder energía hasta, eventualmente, estrellarse contra el núcleo; es decir, conforme a la teoría clásica, el átomo sería inestable. Por tanto, la mecánica que describe los fenónemos atómicos[2] - la Mecánica Cuántica - debe tener como pilares ideas sobre el movimiento distintas a las clásicas.

En el fenómeno de difracción electrónica[3] se ve que al pasar un rayo homogéneo de electrones a través de un cristal, el rayo emergente exhibe un patrón de intensidad notablemente parecido al patrón de difracción descrito por las ondas electromagnéticas. Esta es evidencia de la validez del Principio de de Broglie: "*la materia se comporta de una manera aleatoria y exhibe propiedades típicas de las ondas*".

No podemos predecir exactamente donde estará una partícula a un tiempo futuro así que en Mecánica Cuántica no existe el concepto de camino de una

[2]Por fenómenos atómicos entendemos aquellos donde intervienen partículas cuánticas, es decir, pequeñas masas a pequeñas distancias.

[3]La observación experimental de la difracción electrónica fue posterior a la aparición de la Mecánica Cuántica.

partícula; este es el contenido del **Principio de Incertidumbre**.[4] En todo caso, en un instante determinado, la Mecánica Cuántica debe proveer una distribución probabilística de la posición de la partícula. Más aún, el estado de la partícula a un tiempo $t = t_0$ debe determinar el estado para todo tiempo $t > t_0$; este es el contenido del **Principio de Causalidad**.

La Mecánica Cuántica se presenta como una teoría física bastante inusual pues, por un lado, en las "situaciones cotidianas" debe ser bien aproximada por la Mecánica Clásica (este es el **Principio de Correspondencia**) y, por otra parte, requiere del caso límite, la Mecánica Clásica, para su propia formulación. En efecto, la posibilidad de que alcancemos una descripción cuantitativa del movimiento de una partícula cuántica, digamos un electrón, requiere la presencia de un aparato, esto es, un objeto físico que, bajo un cierto grado de certeza, obedece las leyes de la Mecánica Clásica. Si el electrón interactúa con el aparato (lo que se denomina una medición), el estado de este último se ve alterado. La naturaleza y magnitud de este cambio dependen del estado del electrón y, por tanto, podrían servir para caracterizarlo cuantitativamente. Entonces, el problema que aborda la Mecánica Cuántica consiste en determinar la probabilidad de obtener varios resultados al llevar a cabo una medición.

En Mecánica Cuántica el estado de una partícula es descrito por una función de onda $(\mathbb{R}^d, \mathbb{R}) \ni (x,t) \longmapsto \Psi(x,t) \in \mathbb{C}$. La probabilidad de que una partícula esté en una región $\Omega \subseteq \mathbb{R}^d$ a un tiempo t es $\int_\Omega |\Psi(x,t)|^2 dx$, así que la condición de normalización

$$\int_\Omega |\Psi(x,t)|^2 dx = 1, \quad \forall t \in \mathbb{R}, \tag{2.3}$$

es natural. Si Ψ_1 y Ψ_2 describen la evolución de estados, entonces $\alpha_1\Psi_1 + \alpha_2\Psi_2$, donde α_1 y α_2 son constantes, también describe la evolución de un estado; este es el contenido del **Principio de Superposición de Estados**. Entonces el Espacio de Estados, es decir el conjunto de todos los estados posibles de una partícula a un tiempo dado, será usualmente $\mathrm{L}^2(\mathbb{R}^d)$.

2.3. Magnitudes Físicas y Observables

En Mecánica Clásica, en general, los valores que puede tomar una magnitud física dada forman un espectro continuo. Dicho de otra manera, si una

[4] Descubierto por Heisenberg en 1927.

función $f = f(t)$, representa los cambios de una magnitud física F cuando $t \in [t_0, t_1]$, entonces $f \in \mathrm{C}([t_0, t_1])$. En Mecánica Cuántica, hay también cantidades físicas (e.g. las coordenadas) cuyos valores determinan un rango continuo; sin embargo, a la par de estas, existen también magnitudes cuyo rango de valores admisibles constituyen un espectro discreto. Se denomina cuanto (del latín Quantum, que representa una cantidad de algo) al valor mínimo que puede tomar una determinada magnitud en un sistema físico en el que dicha magnitud esté cuantizada. Esto implica además, que cualquier carga de esa magnitud cuantizada deberá ser un múltiplo entero del cuanto. El ejemplo clásico de un cuanto procede de la descripción de la naturaleza de la luz. Como la energía de la luz está cuantizada, la mínima cantidad posible de energía que puede transportar la luz sería la que proporciona un fotón (nunca se podrá transportar medio fotón). Esta fue una conclusión fundamental obtenida por Max Planck y Albert Einstein en sus descripciones de la ley de emisión de un cuerpo negro y del efecto fotoeléctrico.

En el contexto de la Mecánica Cuántica, no siempre sucede que dos magnitudes físicas dadas pueden ser medidas simultáneamente (e.g. la posición y la velocidad). Por tanto es importante la siguiente

Definición 2.1. A un conjunto de magnitudes físicas tal que sus componentes pueden ser medidos simultáneamente pero que no admiten más esa propiedad si se le añade una magnitud física independiente,[5] se le denomina conjunto completo de magnitudes físicas.

En Física, por "observable" se entiende normalmente una cantidad que puede ser medida experimentalmente. Por otro lado tenemos la siguiente

Definición 2.2. Un observable es, en Mecánica Cuántica, un operador autoadjunto no-acotado[6] con dominio denso en $\mathrm{L}^2(\mathbb{R}^d)$.

Por tanto, los operadores que corresponden (en el formalismo matemático de la Mecánica Cuántica) a cantidades físicas reales tienen que ser observables. En virtud del siguiente teorema (véase [53, Capítulo 1, parágrafe 4]), podemos hablar indistintamente de un conjunto completo de magnitudes físicas o de un conjunto completo de observables.

[5] Aquí por independiente nos referimos a una magnitud que no es una función de las magnitudes bajo consideración inicial.

[6] Una buena referencia para el estudio de los operadores autoadjuntos no-acotados es [64]. Este texto es particularmente útil puesto que los autores tienen siempre en mente los problemas de la Mecánica Cuántica.

Teorema 2.1. *Consideremos los observables* $\hat{f}_1$ *y* $\hat{f}_2$ *correspondientes a las magnitudes físicas* F_1 *y* F_2*. Entonces,* F_1 *y* F_2 *son simultáneamente medibles si y sólo si* $\hat{f}_1$ *y* $\hat{f}_2$ *conmutan, i.e., si y sólo si* $[\hat{f}_1, \hat{f}_2] = 0$.

Corolario 2.1. *Sea* $\{\hat{f}_\alpha\}_{\alpha=1}^N$ *un conjunto de observables asociado a las magnitudes físicas* $\{F_\alpha\}_{\alpha=1}^N$*. Entonces,* $\{F_\alpha\}_{\alpha=1}^N$ *es completo si y sólo si se cumple las siguientes condiciones*

i) $[\hat{f}_\alpha, \hat{f}_\beta] = 0$*, para todo* $\alpha, \beta \in \{1, ..., N\}$,

ii) *si* $\hat{f} \notin \{\hat{f}_\alpha\}_{\alpha=1}^N$ *es un observable, entonces existe* $\alpha_0 \in \{1, ..., N\}$ *tal que* $[\hat{f}, \hat{f}_{\alpha_0}] \neq 0$.

Veamos algunos ejemplos de observables

Ejemplo 2.1. Sea $V : \mathbb{R}^d \longrightarrow \mathbb{R}$ un potencial tal que $\{\Psi \in \mathrm{L}^2(\mathbb{R}^d) : V\Psi \in \mathrm{L}^2(\mathbb{R}^d)\}$ es denso en $\mathrm{L}^2(\mathbb{R}^d)$. Entonces V define un operador de multiplicación

$$\Psi \longmapsto V\Psi \in \mathrm{L}^2(\mathbb{R}^d).$$

Ejemplo 2.2. Al anterior caso pertenece el operador de posición, $\hat{x}$, dado por

$$\Psi \longmapsto x\Psi \in (\mathrm{L}^2(\mathbb{R}^d))^d.$$

Ejemplo 2.3. El operador de momentum, $\hat{p}$, dado por

$$\Psi \longmapsto -i\hbar\nabla\Psi \in (\mathrm{L}^2(\mathbb{R}^d))^d.$$

Aquí cada componente $\hat{p}_i$ de $\hat{p} = (\hat{p}_1, ..., \hat{p}_d)$ es un observable.

Ejemplo 2.4. El operador de Schrödinger

$$\Psi \longmapsto -\frac{\hbar^2}{2m}\Delta\Psi + V(x)\psi \in \mathrm{L}^2(\mathbb{R}^d),$$

donde m es la masa del sistema cuántico y $V = V(x)$ es un potencial dado.

2.4. Sistemas Semi-Clásicos

Por el Principio de Correspondencia, enunciado anteriormente, la Mecánica Clásica debe ser un *límite* de la Mecánica Cuántica. ¿Cómo se da este paso al límite? La respuesta la hallamos con ayuda de la siguiente analogía: la Mecánica Cuántica es a la Mecánica Clásica lo que la Óptica Ondulatoria es a la Óptica Geométrica.

En Óptica Ondulatoria las ondas electromagnéticas son descritas por los campos eléctrico y magnético (que verifican las ecuaciones de Maxwell). Por otro lado, en Óptica Geométrica se considera que la propagación de la luz se da a lo largo de caminos definidos (rayos). Sea $u = v\, e^{i\phi}$ uno de los componentes de campo de la onda electromágnetica, donde v es la *amplitud* y ϕ es la *fase* de la onda. El caso límite, la Óptica Geométrica, corresponde a pequeñas longitudes de onda, esto es, cuando $|\phi|$ es bastante grande.[7] En Óptica Geométrica, el camino de un rayo se determina por el Principio de Fermat, conforme al cual la diferencia entre las fases al principio y fin del camino debe ser la menor posible, ϕ.

De manera similar, supongamos para empezar que a la Mecánica Clásica le corresponde (en Mecánica Cuántica) funciones de onda de la forma $\Psi = v\, e^{i\phi}$, donde v es una función que varía muy poco (en el tiempo) y ϕ es muy grande. Como es sabido, el camino de una partícula en Mecánica Clásica puede ser determinado por el Principio de Mínima Acción, conforme al cual, la *acción* S de un sistema mecánico debe ser la menor posible.

Conforme a la anterior analogía postulamos que la fase de una función de onda debe (al pasar al límite) ser proporcional a la acción mecánica S del sistema considerado: $S = \hbar\phi$. A la constante de proporcionalidad, $\hbar$, se le denomina constante reducida de Planck. Entonces, la función de onda de un Sistema Semi-Clásico viene dada mediante

$$\Psi(x,t) = v(x)e^{iS/\hbar}, \quad (x,t) \in \mathbb{R}^d \times \mathbb{R}. \tag{2.4}$$

Observación 2.1. La constante $\hbar$[8] viene dada en unidades de acción,

$$\hbar = 1{,}0545716818 \times 10^{-34}\; J \cdot s,$$

y juega un rol fundamental en todos los fenómenos cuánticos: su valor relativo (cuando se compara con otras cantidades del sistema dadas en unidades de acción) determina el grado de cuantización del sistema bajo estudio.

[7] En Óptica Geométrica ϕ es llamada la *eikonal*.

[8] La constante de Planck, h, está dada por $h = 2\pi \times \hbar$.

La transición de la Mecánica Cuántica a la Mecánica Clásica puede ser formalmente descrito como el paso al límite cuando $\hbar \longrightarrow 0$. En este proceso, un observable debe reducirse simplemente a la multiplicación por la correspondiente magnitud física.

2.5. La Ecuación de Schrödinger

En Mecánica Cuántica, la función de onda Ψ determina completamente el estado de un sistema físico. Esto quiere decir que si es conocida $\Psi(t_0, \cdot)$, no sólo las propiedades del sistema a $t = t_0$ son conocidas, sino que, el comportamiento en todo $t \geq t_0$ está también determinado.[9] Matemáticamente esto se expresa en que $\partial_t \Psi(t, \cdot)$ debe estar determinado por $\Psi(t, \cdot)$.

En 1925 el Físico austríaco Erwin Schrödinger derivó una ecuación que permite estudiar la evolución de un sistema cuántico. En su versión más general, la Ecuación de Schrödinger toma la forma

$$i\hbar\Psi_t = H\Psi, \tag{2.5}$$

donde el operador H, llamado Hamiltoniano, es el operador asociado a la energía; y, $\Psi(x, t)$ es la función de onda del sistema con la propiedad de que $|\Psi|^2$ determina la distribución de probabilidad de los valores de las coordenadas x (en el espacio de configuración) al tiempo t.

Definición 2.3. A toda solución de (2.5) de la forma (2.4) se le llama estado estacionario (u onda estacionaria) y verifica la *Ecuación de Schrödinger independiente del tiempo*

$$H\psi = E\psi, \tag{2.6}$$

donde E representa la Energía. Al estado estacionario correspondiente al menor de los valores factibles de energía se le conoce como ground state del sistema.[10]. A los estados estacionarios se les refiere como semiclásicos cuando $\hbar > 0$ es chica.

Para el modelo de una única partícula, el Hamiltoniano es un observable muy importante, es el Operador de Schrödinger:

$$H_L = -\frac{\hbar^2}{2m}\Delta + V(x), \tag{2.7}$$

[9]La comprensión de un sistema se entiende hasta donde permiten las limitaciones propias de la Mecánica Cuántica.

[10]Matemáticamente corresponde usualmente a una solución tipo *paso de montaña*

donde m es la masa de la partícula, $V = V(x)$ es un potential dado y $d = 3$. Para ver esto, recurrimos a la formulación (2.4) y recordamos que en el límite cuando $\hbar \longrightarrow 0$, los observables se reducen a multiplicaciones. En efecto, si aplicamos Δ en (2.4) obtenemos

$$\Delta\Psi = -\frac{1}{\hbar^2}|\nabla S|^2\Psi + \frac{i}{\hbar}\Psi\Delta S + e^{iS/\hbar}\left(\Delta v + \frac{i}{\hbar}\nabla v\nabla S\right)$$

que al hacer $\hbar \longrightarrow 0$ nos dice que el operador $-\hbar^2\Delta$ (de la Mecánica Cuántica) se corresponde a la magnitud $|\nabla S|^2$ (de la Mecánica Clásica). Obtenemos (2.7) reemplazando en (2.5) el resultado de derivar en t la relación (2.4), y recurriendo a la Ecuación de Hamilton-Jacobi[11]

$$\partial_t S = -\left(\frac{|\nabla S|^2}{2m} + V(x)\right).$$

Para sistemas cuánticos complejos, sin embargo, el Hamiltoniano resulta de adicionar al operador de Schrödinger una parte no lineal.

Ejemplo 2.5. Para un grupo de partículas idénticas que interactuan entre sí en estados ”ultra—fríos” (e.g. condensados de Bose-Einstein), el proceso evolutivo se describe con un excelente grado de aproximación mediante el Hamiltoniano H_{NL} que está dado por

$$H_{NL}\Psi = -\frac{\hbar^2}{2}\Delta\Psi + V(x)\Psi - |\Psi|^{p-1}\Psi, \tag{2.8}$$

donde m es ahora la masa total del sistema y $p > 1$. Es bastante común $p = 3$ (Ecuación de Gross—Pitaevskii).

2.6. Valor Medio de un Observable

Como se dijo anteriormente, uno de los principios fundamentales de la Mecánica Cuántica es la no-existencia del camino de una partícula. De esto se deduce que no podemos hablar de la velocidad de una partícula a un instante determinado. Sin embargo, se puede recuperar al menos el concepto de velocidad media a través de la siguiente

[11] La ecuación de Hamilton-Jacobi es una de las ecuaciones fundamentales de la Mecánica Clásica.

Definición 2.4. Sea $\hat{L}$ el observable asociado a la magnitud física L. Se define el valor medio de $\hat{L}$ en el estado $\Psi \in \mathrm{dom}(\hat{L})$ como

$$\langle \hat{L} \rangle_\Psi = \Big(\Psi,\, \hat{L}\Psi\Big)_{\mathrm{L}^2(\Omega)}. \tag{2.9}$$

En efecto, consideremos el movimiento de una partícula cuántica. Como se vio anteriormente, el Hamiltoniano está dado por (2.7). Se puede probar (véase e.g. [46]) que para todo observable $\hat{L}$, se tiene que

$$\frac{d}{dt}\langle \hat{L} \rangle_\Psi = \left(\Psi,\, \frac{i}{\hbar}[H_L, \hat{L}]\Psi\right)_{\mathrm{L}^2(\Omega)}. \tag{2.10}$$

Entonces, usando (2.5) y el hecho que $\frac{i}{\hbar}[H_L, \hat{x}] = \frac{1}{m}\hat{p}$, obtenemos (en tanto que valores medios) que el momentum se calcula como el producto de masa por la velocidad:

$$\begin{aligned}
\frac{d}{dt}\langle \hat{x} \rangle_\Psi &= (\partial_t\Psi,\, x\Psi)_{\mathrm{L}^2(\Omega)} + (\Psi,\, x\partial_t\Psi)_{\mathrm{L}^2(\Omega)} \\
&= \left(\Psi,\, \frac{i}{\hbar}[H_L, \hat{x}]\Psi\right)_{\mathrm{L}^2(\Omega)} \\
&= \frac{1}{m}\langle \hat{p} \rangle_\Psi.
\end{aligned}$$

2.7. Representación de Heisenberg

Como se dijo la evolución de un sistema cuántico, ya sea simple o complejo, está definido por la ecuación de Schrödinger (2.5). A esto se refiere usualmente como la representación de Schrödinger.

Sin embargo, históricamente, la Mecánica Cuántica fue primero formulada en la representación de Heisenberg, que corresponde a la evolución de un observable $\hat{L}$. En su forma más general, dicha evolución viene dada por la Ecuación de von Neumann-Heisenberg:

$$i\hbar\partial_t\hat{L}(t) = [H, L(t)], \tag{2.11}$$

donde $\hat{L}(t)$ es un operador de traza, autoadjunto y positivo. Las representaciones de Heisenberg y Schödinger son equivalentes.

Consideremos el caso de una partícula cuántica. Aquí el Hamiltoniano está dado por el operador de Schödinger (2.7). Dado un observable $\hat{L}_0$, definimos

$$\hat{L}(t) = e^{-itH_L/\hbar}\,\hat{L}_0\,e^{itH_L/\hbar}.$$

Sea Ψ la solución de (2.5) con condición inicial $\Psi(\cdot,0) = \Psi_0$, es decir, $\Psi(x,t) = e^{-itH_L/\hbar}\Psi_0(x)$. Entonces, puesto que $e^{-itH_L/\hbar}$ es unitario,

$$\langle \hat{L}_0 \rangle_{\psi(t)} = \langle \hat{L}(t) \rangle_{\psi_0}. \tag{2.12}$$

Ejemplo 2.6. Si ponemos $\hat{L} = \hat{x}$ en (2.11) obtenemos

$$m\,\partial_t x(t) = \hat{p}(t).$$

Si ponemos $\hat{L} = \hat{p}$ en (2.11) obtenemos

$$\partial_t p(t) = -\nabla V \circ \hat{x}(t).$$

Las dos últimas ecuaciones tienen exactamente la misma forma que las Ecuaciones de Hamilton de la Mecánica Clásica.

2.8. El Principio de Incertidumbre

Retomemos la discución sobre el Principio de Incertidumbre. En la Sección 2.2 ya lo enunciamos cualitativamente por lo que ahora nos interesa una manifestación cuantitativa. Para ello consideremos el concepto de dispersión de una magnitud física:

Definición 2.5. Sea $\hat{L}$ el observable asociado a una magnitud física L y sea $\Psi \in \mathrm{dom}(\hat{L}) \subset \mathrm{L}^2(\mathbb{R}^d)$. La dispersión de $\hat{L}$ en el estado Ψ, $\mathrm{disp}_\Psi(\hat{L})$, está dada por

$$\mathrm{disp}^2_\Psi(\hat{L}) = \langle (\hat{L} - \langle \hat{L} \rangle_\Psi)^2 \rangle_\Psi. \tag{2.13}$$

Denotemos por $\hat{x}_j$ y $\hat{p}_j$, respectivamente, el j-ésimo componente de $\hat{x}$ y $\hat{p}$. El Principio de Incertidumbre se expresa entonces en el siguiente

<u>Teorema</u> 2.2. *Se tiene que*

$$disp_\Psi(\hat{x}_j)\; disp_\Psi(\hat{p}_j) \geq \frac{\hbar}{2}, \tag{2.14}$$

para todo $\Psi \in \mathrm{dom}(\hat{x}_j) \cap \mathrm{dom}(\hat{p}_j)$ *y todo* $j = 1, ..., d$.

Demostración. Primero observemos que dados dos observables A y B y $\Psi \in \mathrm{dom}(A) \cap \mathrm{dom}(B)$, se tiene que

$$\langle i[A, B]_\Psi \rangle = -2\mathrm{Im}\,(A\Psi,\, B\Psi)_{\mathrm{L}^2(\Omega)}\,.$$

Por otro lado, se tiene que

$$\frac{i}{\hbar}[\hat{p}_j, \hat{x}_k] = \delta_{jk}, \quad \forall j, k = 1, ..., d.$$

Para simplificar, sin perder generalidad, supongamos que $\langle \hat{x} \rangle_\Psi = \langle \hat{p} \rangle_\Psi = 0$ y que $||\Psi||_{L^2(\mathbb{R}^d)} = 1$. Entonces, para $j = 1, ..., d$,

$$\begin{aligned} 1 &= \left(\Psi,\, \frac{i}{\hbar}[\hat{p}_j, \hat{x}_j]\Psi\right)_{\mathrm{L}^2(\mathbb{R}^d)} \\ &= -\frac{i}{\hbar}\mathrm{Im}(\hat{p}_j\Psi,\, \hat{x}_j\Psi) \\ &\leq \frac{i}{\hbar}||\hat{p}_j\Psi||_{L^2(\mathbb{R}^d)}||\hat{x}_j\Psi||_{L^2(\mathbb{R}^d)} \\ &= \frac{2}{\hbar}\mathrm{disp}_\Psi(\hat{x}_j)\,\mathrm{disp}_\Psi(\hat{p}_j). \end{aligned} \tag{2.15}$$

□

En el siguiente teorema se presenta la desigualdad de Hardy, una versión mejorada del Principio de Incertidumbre.

Teorema 2.3. *Se tiene que*

$$-\Delta \geq \frac{(d-2)^2}{4}\frac{1}{|x|^2}. \tag{2.16}$$

La constante $\frac{(d-2)^2}{4}$ *es optimal.*

Ejemplo 2.7. Como se mencionó al inicio de este capítulo, en Mecánica Clásica los átomos son siempre inestables. Consideremos el átomo de Hidrógeno. Para que sea estable se necesita probar que su único electrón tiene una energía mínima distinta de $-\infty$; pues, en caso contrario, terminaría chocando contra el núcleo. La evolución de este electrón está descrita por el Hamiltoniano $H_0 = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{|x|}$, donde m y e son la masa y la carga del electrón, respectivamente. Aquí $d = 3$. Usando la desigualdad de Hardy se muestra la estabilidad buscada:

$$H_0 = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{|x|} \geq -\frac{2me^4}{\hbar^2}.$$

Capítulo 3

Multiplicidad y concentración para la Ecuación de Schrödinger no-lineal con frecuencia crítica

Como se dijo en la Presentación, mantenemos el idioma en que será publicado el artículo [35]. Los comentarios adicionales serán provistos en notas al pie.

Abstract (*Resumen*)

We consider the nonlinear Schrödinger equation

$$\varepsilon^2 \Delta v - V(x)v + |v|^{p-1}v = 0 \quad \text{in } \mathbb{R}^d, \tag{E}$$

and the limit problem

$$\begin{cases} \Delta u + |u|^{p-1}u = 0, & \text{in} \quad \Omega; \\ u = 0, & \text{on} \quad \partial\Omega \end{cases} \tag{L}$$

where $\Omega = \text{int}\{x \in \mathbb{R}^d : \ V(x) = \text{ínf}\, V = 0\}$ is assumed to be non-empty, connected and smooth. We prove the existence of an infinite number of solutions for (E) and (L) sharing the topology of their level sets, as seen from

the Ljusternik-Schnirelman scheme. Denoting their solutions $\{v_{k,\varepsilon}\}_{k\in\mathbb{N}}$ and $\{u_k\}_{k\in\mathbb{N}}$, respectively, we show that for fixed $k \in \mathbb{N}$ and, up to rescaling $v_{k,\varepsilon}$, the energy of $v_{k,\varepsilon}$ converges to the energy of u_k. It is also shown that the solutions $v_{k,\varepsilon}$ for (E) concentrate exponentially around Ω and that, up to rescaling and up to a subsequence, they converge to a solution of (L).

3.1. Introduction (*Introducción*)

The nonlinear Schrödinger equation, which appears frequently in many fields of physics, typically takes the form[1]

$$i\hbar\Psi_t + \frac{\hbar^2}{2}\Delta\Psi - V_o(x)\Psi + |\Psi|^{p-1}\Psi = 0, \quad \forall x \in \mathbb{R}^d, \forall t \geq 0, \tag{3.1}$$

where $p > 1$ and $\hbar$ denotes the Plank's constant.[2] In this paper we are concerned with the existence and qualitative properties of standing wave solutions of (3.1), that is solutions having the form[3]

$$\Psi(x,t) = v(x) \cdot e^{-iEt/\hbar}.$$

We are specially interested in studying the behavior of the solutions as $\hbar$ approaches zero, that is, in the semi-classical limit.[4] In terms of $v = v(x)$, the problem can be written as

$$\begin{cases} \varepsilon^2\Delta v - V(x)v + |v|^{p-1}v = 0, & \text{in} \quad \mathbb{R}^d; \\ \qquad v(x) \to 0, & \text{as} \quad |x| \longrightarrow \infty \end{cases}, \tag{P_ε}$$

where

$$\begin{cases} \varepsilon^2 = \hbar^2/2, \\ V(x) = V_0(x) - E, \quad x \in \Omega. \end{cases}$$

Here we also assume that $d \geq 3$ and $1 + p \in (2, 2^*)$, with $2^* = \frac{2d}{d-2}$.

There has been an enormous amount of research done in the case where the potential V is assumed to be positive. This research was started in the

[1] Véase el Ejemplo 2.5.
[2] Considérese la Observación 2.1.
[3] Véase la Definición 2.3.
[4] Véase la Sección 2.4

seminal work of Floer and Weinstein [37], where it was shown that in the one dimensional case, for $p = 3$, there is a family of solutions concentrating around a non-degenerate critical point of the potential. These solutions v_ε, which are captured using a Lyapunov-Schmidt reduction method, satisfy

$$\liminf_{\varepsilon\to 0} \max_{x\in\mathbb{R}^d} |v_\varepsilon(x)| > 0. \tag{3.2}$$

Further research and developments have been carried out by many authors, see e.g. Oh [61], Wang [75], Rabinowitz [63], del Pino and Felmer [22], [23], Ambrosetti et al. [1], Gui [43], Li [54], Dancer and Yan [16], Kang and Wei [50] and many others.

In such works, the solutions found satisfy (3.2) and concentrate at certain critical points of the potential, while decaying to zero exponentially, away from them. These works use different approaches, based either on the variational method, or the Lyapunov-Schmidt reduction, or a combination of them. In all these cases, the properties of the positive solutions of the limiting equation are extensively used to obtain the results. In particular, in the Liapunov-Schmidt reduction approach, the uniqueness and non-degeneracy properties of the positive solution of the limit equation are used.

In contrast with the positive-potential case, there are some recent works by Byeon and Wang [11], [12], where they consider a non-negative potential vanishing in a bounded set $\Omega \subset \mathbb{R}^d$. The first important feature is that for the solutions found in [11] and [12], (3.2) does not longer hold; actually the maximum value of the solutions approaches zero. The rates at which these solutions vanish depends on the nature of the set Ω and are certainly strongly related to the nature of the limiting equations. The authors distinguish three cases:

1. $\Omega = \operatorname{int} \overline{\Omega} \neq \emptyset$, which is referred as the *flat case*,
2. $\overline{\Omega}$ is a finite set of points, and V vanishes polynomially at $\overline{\Omega}$, which is referred as the *finite case*, and
3. $\overline{\Omega}$ is a finite set of points, and V vanishes exponentially, which is referred as the *infinite case*.

In this paper we consider the flat case, that is, when the interior of the set $\overline{\Omega}$, where the potential V vanishes, is a non-empty bounded set. In this situation the limiting equation is

$$\begin{cases} \Delta u + |u|^{p-1}u = 0, & \text{in} \quad \Omega; \\ \qquad u = 0, & \text{on} \quad \partial\Omega \end{cases} \tag{P}$$

and, Byeon and Wang proved in [11] that least energy solutions for (P_ε) converges, up to proper scaling, to a least energy solution for (P). Moreover, they showed that the least energy solutions for (P_ε) concentrate in Ω, by proving their exponential decay outside Ω. In the case where Ω has several connected components, the authors can prescribe in which component the concentration will take place. See also the work of Ding and Tanaka [25].

If we further analyze the limiting problem (P) we realize that besides the least energy solutions, there are many more solutions. In particular, the application of the Ljusternik-Schnirelman theory for even functional gives the existence of infinitely many solutions. It is quite natural to ask then if problem (P_ε) has infinitely many solutions and what the relation between them and those of (P) is. In this article we answer this question in the case Ω is connected, we prove that (P_ε) has infinitely many solutions of Ljusternik-Schnirelman type whose critical levels converge to those of (P). Moreover, we prove that these solutions also concentrate in Ω.

Now we present our results in precise terms. We assume that the potential $V(x)$ verifies:

(V1) V is a continuous non-negative function on $\mathbb{R}^d$.

(V2) $V(x) \to \infty$ as $|x| \to \infty$.

(V3) $\Omega = \mathrm{int}\{x \in \mathbb{R}^d \,|\, V(x) = 0\} \neq \emptyset$ is connected and smooth.

We consider the functional

$$J_\varepsilon(w) = \frac{1}{2}\int_{\mathbb{R}^d} \left(|\nabla w|^2 + \frac{1}{\varepsilon^2}V(x)w^2 \right) dx, \tag{3.3}$$

defined on

$$\mathcal{M}_\varepsilon = \{w \in H_\varepsilon : \, ||w||_{L^{p+1}(\mathbb{R}^d)} = 1\},$$

where

$$H_\varepsilon \equiv \left\{ w \in \mathrm{H}^1(\Omega) : \, ||w||_\varepsilon \equiv \left(\int_{\mathbb{R}^N} |\nabla w|^2 + \frac{V(x)}{\varepsilon^2} w^2 \right)^{1/2} < \infty \right\}.$$

The critical points of J_ε on $\mathcal{M}_\varepsilon$ give rise, via scaling, to the solutions of (P_ε).

In our context, the flat case of Byeon and Wang in [11], the limit equation for (P_ε) is (P). Associated to (P) we consider the functional

$$J(u) = \frac{1}{2}\int_\Omega |\nabla u|^2 dx, \tag{3.4}$$

defined on

$$\mathcal{M} = \{u \in \mathrm{H}_0^1(\Omega) : \ ||u||_{L^{p+1}(\Omega)} = 1\}.$$

The critical points of J on $\mathcal{M}$ are, up to scaling, the solutions of (P).

Remark 3.1. A family of functions $\{f_\varepsilon\}_{\varepsilon>0}$ is said to sub-converge in a space X, as $\varepsilon \to 0$, when from any sequence $\{\varepsilon_i\}_{i\in\mathbb{N}}$ converging to zero it is possible to extract a subsequence $\{\varepsilon_{n_i}\}_{i\in\mathbb{N}}$ such that $\{f_{\varepsilon_{n_i}}\}_{i\in\mathbb{N}}$ converge in X, as $i \to \infty$.

Let state our main result:

Theorem 3.1. *Under our general assumptions on the potential (V1), (V2) and (V3), and assuming that $d \geq 3$ and $1 < p < (d+2)/(d-2)$ we have:*

- ***i)*** *Given $\varepsilon > 0$ the functional J_ε possesses infinitely many critical points $\{\hat{w}_{k,\varepsilon}\}_{k\in\mathbb{N}} \subset \mathcal{M}_\varepsilon$.*
- ***ii)*** *The limit functional J has infinitely many critical points $\{\hat{w}_k\}_{k\in\mathbb{N}} \subset \mathcal{M}$.*
- ***iii)*** *Given $k \in \mathbb{N}$, the critical values satisfy*

$$\lim_{\varepsilon\to 0} J_\varepsilon(\hat{w}_{k,\varepsilon}) = J(\hat{w}_k). \tag{3.5}$$

- ***iv)*** *Moreover, given $\delta, c > 0$, there exists $\varepsilon_0 > 0$ such that*

$$|\hat{w}_{k,\varepsilon}(x)| < C \cdot \exp\{-\frac{c}{\varepsilon} \cdot \mathrm{dist}(x, \Omega^\delta)\}, \quad \forall x \in \mathbb{R}^d,\ \forall \varepsilon \in]0, \varepsilon_0), \tag{3.6}$$

where $C > 0$ and $\Omega^\delta = \{x \in \mathbb{R}^d : \ \mathrm{dist}(x, \Omega) < \delta\}$.

- ***v)*** *On the boundary of Ω, the functions $\hat{w}_{k,\varepsilon}$ verify*

$$\lim_{\varepsilon\to 0} \max_{x\in\partial\Omega} |\hat{w}_{k,\varepsilon}(x)| = 0, \quad \forall k \in \mathbb{N}. \tag{3.7}$$

Remark 3.2. It's clear that the functions

$$v_{k,\varepsilon} = (2\varepsilon^2 c_{k,\varepsilon})^{1/(p-1)} \hat{w}_{k,\varepsilon}, \qquad c_{k,\varepsilon} = J_\varepsilon(\hat{w}_{k,\varepsilon})$$

are solutions of (P_ε) and, as a corollary, they satisfy, for fixed $k \in \mathbb{N}$,

$$\lim_{\varepsilon\to 0} ||v_{k,\varepsilon}||_{L^\infty(\mathbb{R}^d)} = 0 \tag{3.8}$$

and

$$\liminf_{\varepsilon\to 0} \frac{||v_{k,\varepsilon}||_{L^\infty(\mathbb{R}^d)}}{\varepsilon^{2/(p-1)}} > 0. \tag{3.9}$$

It's not hard to see that the functions $w_{k,\varepsilon} = (2c_{k,\varepsilon})^{1/(p-1)} \hat{w}_{k,\varepsilon}$ satisfy the equation

$$\begin{cases} \Delta w - \varepsilon^{-2} V(x) w + |w|^{p-1} w = 0, & \text{in} \quad \mathbb{R}^d; \\ \qquad w(x) \to 0, & \text{as} \quad |x| \longrightarrow \infty \end{cases} \tag{P'_ε}$$

We prove, for every k, the existence of a subsequence of $w_{k,\varepsilon}$ converging to w_k, a solution of (P).

The behaviour described for our sequence of solutions corresponds to the same phenomena discussed by Byeon and Wang, ([11, Th.2.2]), for (positive) least energy solutions. Property (3.8) is in contrast to the non-critical case, $\inf_{x\in\mathbb{R}^d} V(x) > 0$, where all the solutions of (P_ε) are bounded away from zero.

In [11] it is shown that the rescaled function $w_\varepsilon = \varepsilon^{-2/(p-1)} v_\varepsilon$ sub-converges point-wise to a least energy solution U of (P), in Ω, and to 0 in $\mathbb{R}^d \setminus \Omega$. Moreover, given $\delta > 0$, the convergence is uniform on $\{x \in \mathbb{R}^d : \text{dist}(x, \partial\Omega) \geq \delta\}$.

Remark 3.3. The potential considered in this article is non-negative and vanishing at an open set Ω. This situation is considered critical since the limiting behavior of solutions is quite different. For the positive-potential case, least energy solutions must concentrate at a point, however for a vanishing potential the concentration occurs at the whole set Ω. When the potential becomes negative in a bounded set, then least energy solutions no longer makes sense. However, this situation can still be well understood, at least in the one dimensional case, and in the radial case, as in the work by Felmer and Torres [36] and Castro and Felmer [15], respectively.

Remark 3.4. We do not say anything about the sign of the solutions we found; however, since the limit problem (P) may have many positive solutions depending on the geometry of Ω (see e.g. [17]), the same could happen with (P_ε).

Remark 3.5. In this article we consider only the case of a potential diverging to infinity as $|x| \to \infty$, that is satisfying (V2), and vanishing in a connected, open, smooth set, that is satisfying (V3). We think that our results hold for more general potentials, when the zero set of V is not connected, and also for the finite and infinite cases. Particularly challenging may be the case of a bounded potential, positive at infinity. In this case the existence of infinitely many critical points as in Theorem 1.1, i) may be no longer true. However, the statements, ii)-v), with k fixed, should be true.

Actually, after we finished this article, we learned of a recent work of Ding and Szulkin [24] where this problem is treated. Instead of conditions (V2) and (V3) they assume that

(V2') there exists $b > 0$ such that the set $\{x \in \mathbb{R}^d : V(x) < b\}$ is nonempty and has finite measure.

Fixed $k \in \mathbb{N}$, they prove that for some $\Lambda_k > 0$, problem (P_ε) has at least k pairs of solutions in H_ε when $\varepsilon \in]0, \Lambda_k^{-1/2}[$. In contrast we prove the existence of an infinite number of solutions, at least a pair for each level of energy. If, for every $m \in \mathbb{N}$, u_m is a solution of (P_{ε_m}), where $\text{lím}_{m\to\infty} \varepsilon_m = 0$, then they show that u_m converges in H_1 to some solution u of (P) assuming the boundedness of $(||u_m||_{\varepsilon_m})_{m\in\mathbb{N}}$. In Lemma 3.1 we prove this last condition for each level k of energy and, in Lemma 3.6, we prove that our solutions $(w_{k,\varepsilon})$ subconverge in $\mathrm{H}^1(\Omega)$ to some solution of (P).

We observe that as far as the existence and the number of solutions are concerned, the problem

$$\begin{cases} \Delta v - V_\lambda(x)v + |v|^{p-1}v = 0, & \text{in} \quad \mathbb{R}^d; \\ \qquad v(x) \to 0, & \text{as} \quad |x| \longrightarrow \infty \end{cases}, \tag{P_λ}$$

where $V_\lambda = \lambda V$, is equivalent to (P_ε). In fact, putting $\varepsilon^2 = \lambda^{-1}$, it is clear that u is a solution of (P_λ) if and only if $v = \lambda^{-1/(p-2)}u$ is a solution of (P_ε). In some recent work, Bartsch and Wang [5] and Bartsch et al. [4] dealt with problem (P_λ) when $V_\lambda(x) = a_0(x) + \lambda a(x)$, where $a_0 \in \mathrm{L}^\infty(\mathbb{R}^d)$ is bounded away from zero, and $a \in L^\infty(\mathbb{R}^d)$ is non-negative and such that for some $M_0 > 0$ and some $Z = \overline{Z} \subset \mathbb{R}^d$ with non-empty interior,

$$a(x) = 0, \quad \forall x \in Z \qquad \text{and} \qquad a(x) > 0, \quad a.e.\, x \in Z^c,$$

and

$$|\{x \in \mathbb{R}^d : \ a(x) < M_0\}| < \infty.$$

They show that for every integer $k \in \mathbb{N}$, there exists Λ_k such that (P_λ) has at least k pairs of (weak) solutions when $\lambda > \Lambda_k$; with additional conditions these solutions have exponential decay at infinity. They prove that a sequence $\{u_n\}_{n\in\mathbb{N}}$ of solutions for (P_{λ_n}), $\lambda_n \longrightarrow \infty$, converge in $H^1(\Omega)$ to a solution of

$$\begin{cases} -\Delta u + a_0(x)u = |u|^{p-1}, & \text{in int } Z, \\ \qquad\qquad u = 0, & \text{in } Z^c, \end{cases}$$

provided the uniform boundedness of the energy norms of $\{u_n\}_{n\in\mathbb{N}}$ and $\text{ínf}_n ||u_n||_{L^p(\mathbb{R}^d)} > 0$.

We finally mention that in our work we not only obtain exponential decay of the solutions at infinity, but we get further asymptotic estimates on their behavior on the boundary of the domain.[5]

We devote this paper to prove Theorem 3.1. In Section 3.2 we set up the Ljusternik-Schnirelman scheme to prove parts i) and ii) of Theorem 1.1. In Section 3.3, we study the asymptotic behavior of the critical values proving iii) of Theorem 3.1. In section 3.4 we analyze the decay of the solutions away from Ω and in Section 3.5 we study the behavior on the boundary, proving iv) and v), respectively.

3.2. Ljusternik-Schnirelman setting: Multiplicity (*Multiplicidad via un esquema de Ljusternik-Schnirelman*)

In this section we set up the Ljusternik-Schnirelman scheme in order to prove the first two statements in Theorem 3.1.

[5] Véase la Sección 3.5.

In general terms, given a Banach space E, we write

$$\Sigma_E = \{A \subset E : \ A = \overline{A}, \, A = -A, \, 0 \notin A\}$$

and consider on Σ_E the Krasnoselski's genus γ.[6] The following theorem is proved in [62]

<u>Theorem</u> 3.2. *Let $M \in \Sigma_E$ be C^1 sub-manifold of E and let $f \in \mathrm{C}^1(E)$ be even. Suppose that (M,f) satisfy the Palais-Smale condition and let*

$$C_k(f) = \inf_{A \in \mathcal{A}_k(M)} \max_{u \in A} f(u), \tag{3.10}$$

where

$$\mathcal{A}_k(M) = \{A \in \Sigma_E \cap M : \ \gamma(A) \geq k\}. \tag{3.11}$$

If $C_k(f) \in \mathbb{R}$, then $C_k(f)$ is a critical value for f. Moreover, if $c \equiv C_k(f) = ... = C_{k+m}(f)$, then $\gamma(K_c) \geq m+1$. In particular, if $m > 1$, then K_c, the set of critical points corresponding to the value c, contains infinitely many elements.

It is clear that the functional (3.4) verifies the conditions of Theorem 3.2. Then we write $\Sigma = \Sigma_{\mathrm{H}_0^1(\Omega)}$, and for each $k \in \mathbb{N}$,

$$\mathcal{A}_k = \mathcal{A}_k(\mathcal{M}) \quad \text{and} \quad c_k = C_k(J) = J(\hat{w}_k) \in (0, \infty).$$

Remark 3.6. With this it is clear that

$$w_k \equiv (2c_k)^{1/(p-1)} \cdot \hat{w}_k$$

is a solution of (P).

In our study it will be convenient to have an intermediate problem. Given $\delta > 0$ we write $\Omega^\delta = \{x \in \mathbb{R}^d : \ \mathrm{dist}(x, \Omega) < \delta\}$, and consider the problem

$$\begin{cases} \Delta u + |u|^{p-1} u = 0, & \text{in} \quad \Omega^\delta; \\ \qquad u = 0, & \text{on} \quad \partial\Omega^\delta \end{cases} \tag{P^δ}$$

with the functional

$$J^\delta(u) \equiv \frac{1}{2} \int_{\Omega^\delta} |\nabla u|^2 dx. \tag{3.12}$$

[6]Para el género de Krasnoselsi y la condición de Palais-Smale véase [62].

defined on

$$\mathcal{M}^\delta = \{u \in \mathrm{H}_0^1(\Omega^\delta) : \ ||u||_{L^{p+1}(\Omega^\delta)} = 1\}.$$

Here we write $\Sigma^\delta = \Sigma_{\mathrm{H}_0^1(\Omega^\delta)}$, and for each $k \in \mathbb{N}$

$$\mathcal{A}_k^\delta = \mathcal{A}_k(\mathcal{M}^\delta) \quad \text{and} \quad c_k^\delta = C_k(J^\delta) = J^\delta(\hat{w}_k^\delta) \in (0, +\infty).$$

It is clear that the function $w_k^\delta = (2c_k^\delta)^{1/(p-1)}\hat{w}_k^\delta$ is a solution of (P^δ).

Theorem 3.2 can also be applied to (P_ε). In fact, the compactness of the embedding $H_\varepsilon \subset \mathrm{L}^q(\mathbb{R}^d)$, $q \in [2, 2^*)$, can be proved applying the Fréchet - Kolmogorov theorem ([9, Cor. IV.26]); and with this, it is proved that the corresponding functional is C^1 and satisfies the Palais-Smale condition in the manifold $\mathcal{M}_\varepsilon$. We put

$$\Sigma_\varepsilon = \Sigma_{H_\varepsilon}, \quad \forall \varepsilon > 0,$$

and, for every $k \in \mathbb{N}$ and every $\varepsilon > 0$,

$$\mathcal{A}_{k,\varepsilon} = \mathcal{A}_k(\mathcal{M}_\varepsilon) \quad \text{and} \quad c_{k,\varepsilon} = C_k(J_\varepsilon) = J_\varepsilon(\hat{w}_{k,\varepsilon}).$$

Remark 3.7. With this it is clear that

$$v_{k,\varepsilon} = (2\varepsilon^2 c_{k,\varepsilon})^{1/(p-1)} \cdot \hat{w}_{k,\varepsilon}$$

is a solution of (P_ε) and

$$w_{k,\varepsilon} \equiv (2c_{k,\varepsilon})^{1/(p-1)} \cdot \hat{w}_{k,\varepsilon}$$

is a solution of (P'_ε).

Remark 3.8. Assuming further that the potential is of class C^α, using the well-known regularity theory, it can be proved that each 'solution' which appears in this paper is a classical one and belongs to the class $\mathrm{C}^{2,\alpha}$.

3.3. Limits for the Critical Values (*Límites de los Valores Críticos*)

This section is devoted to prove iii) of Theorem 1.1. As discussed in the last section, the multiplicity result is based on the Ljusternik-Schnirelman theory for even functional. The index k of the critical values, represent the topological characteristic of the level set, as captured by the Krasnoselski genus.

Thus, our main result in this section corresponds to proving that the level sets of J_ε and J for the Ljusternik-Schnirelman values are topologically equivalent. Actually we prove

Theorem 3.3. *For every $k \in \mathbb{N}$, we have*

$$\lim_{\varepsilon \to 0} c_{k,\varepsilon} = c_k. \tag{3.13}$$

The proof of this theorem is divided in several steps as given by the following lemmas.

Lemma 3.1. *For every $k \in \mathbb{N}$ and every $\varepsilon > 0$, we have*

$$c_{k,\varepsilon} \leq c_k. \tag{3.14}$$

Proof. If we identify each $u \in \mathrm{H}_0^1(\Omega)$ with its extension by zero outside Ω then we have $\mathrm{H}_0^1(\Omega) \subset H_\varepsilon$. We also have that $||u||_\varepsilon = ||u||_{H_0^1(\Omega)}$, for all $u \in \mathrm{H}_0^1(\Omega)$, and clearly $\mathcal{A}_k \subset \mathcal{A}_{k,\varepsilon}$. Hence $c_{k,\varepsilon} \leq c_k$, for every $k \in \mathbb{N}$. □

Now the crucial lemma

Lemma 3.2. *Let $k \in \mathbb{N}$ and $\sigma > 0$. Given $\delta > 0$ small, there exists a $\varepsilon_\delta > 0$ such that*

$$c_k^\delta \leq c_{k,\varepsilon} + \sigma, \tag{3.15}$$

for every $\varepsilon \in (0, \varepsilon_\delta)$.

Proof. According to the definition of the $c_{k,\varepsilon}$, given $\varepsilon > 0$ (in principle without restrictions), we choose $A_\sigma(\varepsilon) \in \mathcal{A}_{k,\varepsilon}$ in such a way that

$$\max_{v \in A_\sigma(\varepsilon)} J_\varepsilon(v) \leq c_{k,\varepsilon} + \frac{\sigma}{3} \tag{3.16}$$

holds. Then, by Lemma 3.1,

$$J_\varepsilon(v) \leq c_k + \frac{\sigma}{3} \equiv b_{k,\sigma}, \quad \forall v \in A_\sigma(\varepsilon). \tag{3.17}$$

From here we directly obtain that

$$\frac{1}{2} \int_{\mathbb{R}^d} |\nabla v|^2 \leq b_{k,\sigma}, \quad \forall v \in A_\sigma(\varepsilon) \tag{3.18}$$

and

$$b_{k,\sigma} \geq \frac{1}{2} \int_{\mathbb{R}^d \setminus \Omega} \frac{V(x)}{\varepsilon^2} v^2 \geq \frac{1}{2} \int_{\mathbb{R}^d \setminus \Omega^\delta} \frac{V(x)}{\varepsilon^2} v^2, \tag{3.19}$$

for all $v \in A_\sigma(\varepsilon)$ and all $\delta > 0$. Here we notice that the constant $b_{k,\sigma}$ does not depend on ε. Now, putting

$$V_\rho \equiv \inf_{x \in \mathbb{R}^d \setminus \Omega^\rho} V(x),$$

we have

$$||v||_{L^2(\mathbb{R}^d \setminus \Omega^\delta)} \leq \left(\frac{2b_{k,\sigma}}{V_\delta} \right)^{1/2} \varepsilon, \qquad \forall \delta > 0, \forall v \in A_\sigma(\varepsilon). \tag{3.20}$$

From (3.18) and using the Sobolev-Gagliardo-Nirenberg inequality we get

$$||v||_{L^{2^*}(\mathbb{R}^d)} \leq C b_{k,\sigma}^{1/2}, \quad \forall v \in A_\sigma(\varepsilon), \tag{3.21}$$

for some constant C. Thus, we conclude

$$\lim_{\varepsilon \to 0} \max_{v \in A_\sigma(\varepsilon)} ||v||_{L^{p+1}(\mathbb{R}^d \setminus \Omega^\delta)} = 0, \quad \forall \delta > 0. \tag{3.22}$$

In fact, getting $\alpha \in (0,1)$ such that $\frac{1}{p+1} = \frac{(1-\alpha)}{2} + \frac{\alpha}{2^*}$, it follows by interpolation, considering (3.20) and (3.21), that

$$||v||_{L^{p+1}(\mathbb{R}^d \setminus \Omega^\delta)} \leq \eta \varepsilon^{1-\alpha}, \quad \forall v \in A_\sigma(\varepsilon), \forall \delta > 0, \tag{3.23}$$

with

$$\eta = \eta(\delta, k, \sigma, q) = C \left(\frac{b_{k,\sigma}}{V_\delta^{1-\alpha}} \right)^{1/2}.$$

From (3.22) it is clear that, given $\delta > 0$ and $s > 0$, we can get a $\varepsilon_1 = \varepsilon_1(\delta, s) > 0$ such that

$$\max_{v \in A_\sigma(\varepsilon)} ||v||_{L^{p+1}(\mathbb{R}^d \setminus \Omega^\delta)} \leq \delta^s, \quad \forall \varepsilon \in (0, \varepsilon_1[\tag{3.24}$$

and thus, in particular for $s = 1$,

$$||v||_{L^{p+1}(\Omega^\delta)} \geq 1 - \delta, \quad \forall v \in A_\sigma(\varepsilon), \forall \varepsilon \in (0, \varepsilon_1[, \forall \delta > 0. \tag{3.25}$$

From now on we will assume that $0 < \delta < 1$. We choose a cut-off function $\phi_\delta \in C_0^\infty(\Omega)$ such that $\phi_\delta \equiv 1$ in $\Omega^{\delta/2}$ and $\phi_\delta \equiv 0$ in $\mathbb{R}^d \setminus \Omega^\delta$,

$$0 < \phi_\delta(x) < 1 \quad \text{and} \quad |\nabla \phi_\delta(x)| \leq \frac{1}{\delta^r} \quad \forall x \in \Omega^\delta \setminus \overline{\Omega^{\delta/2}}, \tag{3.26}$$

for some $r > 1$.

Now we define for $u \in \mathcal{M}_\varepsilon$

$$\phi_\delta[u] \equiv \frac{\phi_\delta u}{||\phi_\delta u||_{L^{p+1}(\mathbb{R}^d)}}, \tag{3.27}$$

and we claim that

$$\phi_\delta[A_\sigma(\varepsilon)] \in \mathcal{A}_k^\delta, \quad \forall \varepsilon \in (0, \varepsilon_1). \tag{3.28}$$

In fact, as a consequence of the concentration property given in (3.25), for all $v \in A_\sigma(\varepsilon)$ and all $\varepsilon \in (0, \varepsilon_1)$,

$$\int_{\Omega^\delta} |\phi_\delta v|^{p+1} = \int_{\Omega^{\delta/2}} |v|^{p+1} + \int_{\Omega^\delta \setminus \Omega^{\delta/2}} |\phi_\delta v|^{p+1} \geq (1 - \frac{\delta}{2})^{p+1}, \tag{3.29}$$

so that

$$||\phi_\delta v||_{L^{p+1}(\Omega^\delta)} \geq 1 - \delta, \tag{3.30}$$

and in particular we see that $\phi_\delta[\cdot]$ is well defined and we further conclude that it is continuous. Then, since $\phi_\delta[\cdot]$ is odd, from genus properties we have that

$$\gamma(\phi_\delta[A_\sigma(\varepsilon)]) \geq k, \quad \forall\, \varepsilon \in (0, \varepsilon_1).$$

Hence, considering (3.28) and the definition of c_k^δ, we get

$$c_k^\delta \leq \max_{v \in \phi_\delta[A_\sigma(\varepsilon)]} J^\delta(v), \quad \forall \varepsilon \in (0, \varepsilon_1). \tag{3.31}$$

Let us take now an element $u \in A_\sigma(\varepsilon)$ such that $\bar{v} \equiv \phi_\sigma[u]$ satisfies

$$\max_{v \in \phi_\delta[A_\sigma(\varepsilon)]} J^\delta(v) \leq J^\delta(\bar{v}) + \frac{1}{3}\sigma. \tag{3.32}$$

At this stage, we observe that in order to complete the proof of the lemma it is enough to prove the existence of an element $w \in A_\sigma(\varepsilon)$ satisfying

$$J^\delta(\bar{v}) \leq J_\varepsilon(w) + \frac{1}{3}\sigma. \tag{3.33}$$

In fact, from (3.16), (3.31), (3.32) and (3.33), we have

$$c_k^\delta \leq J^\delta(\bar{v}) + \frac{1}{3}\sigma \leq J_\varepsilon(w) + \frac{2}{3}\sigma \leq \max_{u\in A_\sigma(\varepsilon)} J_\varepsilon(u) + \frac{2}{3}\sigma \leq c_{k,\varepsilon} + \sigma.$$

We devote the rest of the proof to find such a w. For $\bar{v} = \phi_\sigma[u]$, a direct computation gives

$$\begin{aligned}\|\phi_\delta u\|^2_{L^{p+1}(\mathbb{R})} J^\delta(\bar{v}) &\leq \int_{\Omega^\delta} u^2|\nabla\phi_\delta|^2 + 2u\phi_\delta\nabla u\nabla\phi_\delta + \phi_\delta^2|\nabla u|^2 \\ &\leq \int_{\Omega^\delta} u^2|\nabla\phi_\delta|^2 + 2u\phi_\delta\nabla u\nabla\phi_\delta + \int_{\mathbb{R}^d} |\nabla u|^2 + \frac{V(x)}{\varepsilon^2}u^2\end{aligned}$$

whence

$$\begin{aligned}(1-\delta)^2 J^\delta(\bar{v}) &\leq J_\varepsilon(u) + \int_{\Omega^\delta\setminus\overline{\Omega^{\delta/2}}} u^2|\nabla\phi_\delta|^2 + 2u|\nabla u||\nabla\phi_\delta| \\ &\leq J_\varepsilon(u) + \frac{1}{\delta^{2r}}\int_{\Omega^\delta\setminus\overline{\Omega^{\delta/2}}} u^2 + \frac{2}{\delta^r}\int_{\Omega^\delta\setminus\overline{\Omega^{\delta/2}}} u|\nabla u| \\ &\leq J_\varepsilon(u) + \frac{C}{\delta^{2r}}\left(\int_{\Omega^\delta\setminus\overline{\Omega^{\delta/2}}} u^2\right)^{1/2}\end{aligned}$$

where we have used (3.26), (3.30), (3.3), (3.18) and the Cauchy-Schwartz inequality. We observe that the constant C depends on k through $b_{k,\sigma}$. Then, using Hölder inequality, considering (3.24) and taking $s > 2r$, we get (decreasing ε_1 if necessary) that

$$(1-\delta)^2 J^\delta(\bar{v}) \leq J_\varepsilon(u) + C\delta^{s-2r}, \quad \forall\varepsilon \in (0,\varepsilon_1). \tag{3.34}$$

Here, if $\delta \in (0, \frac{1}{4})$ then $\frac{1}{2}J^\delta(\bar{v}) \leq J_\varepsilon(u) + C\delta^{s-2r} \leq b_{k,\sigma} + C\delta^{s-2r}$. So, from (3.34) we get

$$J^\delta(\bar{v}) \leq J_\varepsilon(u) + C\delta^{s-2r} + 2\delta(b_{k,\sigma} + C\delta^{s-2r}).$$

From here we obtain (3.33) putting $u = w$ when $\delta \in (0, \frac{1}{4})$ is small enough and $\varepsilon \in (0, \varepsilon_1)$. □

Lemma 3.3. *Given $k \in \mathbb{N}$ and $\delta > 0$, we have*

$$c_k^\delta \leq c_k.$$

Proof. We identify each $u \in \mathrm{H}_0^1(\Omega)$ with its extension by zero to $\Omega^\delta \backslash \overline{\Omega}$. In this sense we have $\mathrm{H}_0^1(\Omega) \subset \mathrm{H}_0^1(\Omega^\delta)$ and $||u||_{H_0^1(\Omega^\delta)} = ||u||_{H_0^1(\Omega)}$, for all $u \in \mathrm{H}_0^1(\Omega)$. Thus, it is clear that $\mathcal{A}_k \subset \mathcal{A}_k^\delta$ and then $c_k^\delta \leq c_k$, for every $k \in \mathbb{N}$. □

Lemma 3.4. *Given $k \in \mathbb{N}$ and $\sigma > 0$, there exists $\delta_\sigma > 0$ such that*

$$c_k \leq c_k^\delta + \sigma,$$

for every $\delta \in (0, \delta_\sigma)$.

Proof. According to the definition of c_k^δ, given $\delta > 0$ we may choose $B_\sigma(\delta) \in \mathcal{A}_k^\delta$ such that

$$\max_{v \in B_\sigma(\delta)} J^\delta(v) \leq c_k^\delta + \frac{\sigma}{3}. \tag{3.35}$$

Then, from Lemma 3.3, we get

$$J^\delta(v) \leq c_k + \frac{\sigma}{3} \equiv b_{k,\sigma}, \quad \forall v \in B_\sigma(\delta). \tag{3.36}$$

Now we choose a $\delta_0 = \delta_0(\Omega) > 0$ so that for every $\delta \in (0, \delta_0)$ we can associate a diffeomorphism $\psi_\delta = (\psi_\delta^{(1)}, ..., \psi_\delta^{(d)}) \in \mathrm{C}^1(\overline{\Omega}; \overline{\Omega^\delta})$ such that

$$|\psi_\delta(x) - x| \leq O(\delta) \quad \text{and} \quad |D\psi_\delta(x) - I^d| \leq O(\delta) \quad \forall x \in \overline{\Omega}, \tag{3.37}$$

and

$$\psi_\delta(\partial\Omega) = \partial\Omega^\delta. \tag{3.38}$$

Here I^d denotes the $d \times d$ identity matrix. Now we define the application $\Gamma_\delta[\cdot] : \mathrm{H}_0^1(\Omega^\delta) \to \mathrm{H}_0^1(\Omega)$ as

$$\Gamma_\delta[v](x) = \frac{v \circ \psi_\delta(x)}{||v \circ \psi_\delta||_{L^{p+1}(\Omega)}}, \qquad x \in \Omega,$$

for all $v \in \mathrm{H}_0^1(\Omega^\delta) \setminus \{0\}$. We claim that there exists $\delta_1 \in (0, \delta_0)$ such that

$$\Gamma_\delta[B_\sigma(\delta)] \in \mathcal{A}_k, \quad \forall \delta \in (0, \delta_1). \tag{3.39}$$

We see that in order to prove (3.39) it suffices to show that Γ_δ is well defined and continuous, since clearly Γ_δ is odd. We do this now.

First, we observe that from (3.37), for every $\eta > 0$, there exists a $\delta_2 = \delta_2(\eta) > 0$, $\delta_2 \leq \delta_1$, such that

$$1 - \eta \leq \det D\psi_\delta(x) \leq 1 + \eta, \quad \forall x \in \overline{\Omega}, \forall \delta \in (0, \delta_2). \tag{3.40}$$

From now on we assume that $\delta \in (0, \delta_2)$. Let v be an arbitrary element in $\mathrm{H}_0^1(\Omega^\delta) \setminus \{0\}$. Then, from (3.40) and the formula of change of variables we get

$$\begin{aligned} ||v \circ \psi_\delta||_{L^{p+1}(\Omega)}^{p+1} &\geq |1+\eta|^{-1} \int_\Omega |v \circ \psi_\delta|^{p+1} \det D\psi_\delta(x) \\ &\geq |1+\eta|^{-1} \int_{\Omega^\delta} |v|^{p+1}. \end{aligned}$$

Thus, in particular $v \circ \psi_\delta \neq 0$, for every $v \in \mathrm{H}_0^1(\Omega^\delta)$. Using again (3.40) we obtain that for all $v \in \mathrm{H}_0^1(\Omega^\delta) \setminus \{0\}$

$$\frac{||v||_{L^{p+1}(\Omega^\delta)}}{|1+\eta|^{1/(p+1)}} \leq ||v \circ \psi_\delta||_{L^{p+1}(\Omega)} \leq \frac{||v||_{L^{p+1}(\Omega^\delta)}}{|1-\eta|^{1/(p+1)}}.$$

Let us prove next that

$$\Gamma_\delta(v) \in \mathrm{H}_0^1(\Omega) \setminus \{0\}, \quad \forall v \in \mathrm{H}_0^1(\Omega^\delta) \setminus \{0\}. \tag{3.41}$$

Let $i \in \{1, ..., N\}$ and $w \in \mathrm{C}_0^\infty(\Omega^\delta) \setminus \{0\}$ then we have

$$D_i \Gamma_\delta[w](x) = \frac{\sum_{j=1}^N g_{i,j}(x)}{||w \circ \psi_\delta||_{L^{p+1}(\Omega)}}, \qquad x \in \overline{\Omega},$$

where $g_{i,j}(x) = D_j w(\psi_\delta(x)) \cdot D_i \psi_\delta^{(j)}(x)$. Then, from (3.40) and using the formula of change of variables again, we get

$$\begin{aligned} \int_\Omega \left| \sum_{j=1}^N g_{i,j}(x) \right|^2 &\leq \int_{\psi_\delta^{-1}(\Omega^\delta)} \sum_{j=1}^N |g_{i,j}(x))|^2 \frac{\det D\psi_\delta(x)}{\det D\psi_\delta(x)} \\ &\leq C \int_{\Omega^\delta} \sum_{j=1}^N |D_j w|^2, \end{aligned}$$

where $C = (1-\eta)^{-1} \left(\text{máx}_{\substack{x \in \Omega \\ j=1,\ldots,N}} \left| D_i \psi_\delta^{(j)}(x) \right|^2 \right)$. Moreover, from (3.38) we have $\Gamma_\delta[w]|_{\partial\Omega} = 0$ and then $\Gamma_\delta[w] \in \mathrm{H}_0^1(\Omega)$. Thus we have proved that $\Gamma_\delta[w] \in \mathrm{H}_0^1(\Omega) \setminus \{0\}$ and

$$||\Gamma_\delta(w)||_{H_0^1(\Omega)} \leq K ||w||_{H_0^1(\Omega^\delta)}, \quad \forall w \in \mathrm{C}_0^\infty(\Omega^\delta), \tag{3.42}$$

for certain $K = K(\eta, \delta, N)$. Using a density argument we extend this inequality to all $H_0^1(\Omega^\delta)$. From here we obtain (3.41) and the continuity of $\Gamma_\delta[\cdot]$. Finally, from (3.41) and (3.42), we obtain (3.39) proving the claim.

Now, considering (3.39) and the definition of c_k, it follows that

$$c_k \leq \max_{u \in \Gamma_\delta[B_\sigma(\delta)]} J(u). \tag{3.43}$$

On the other hand, let us take $v \in B_\sigma(\delta)$ such that $u = \Gamma_\delta[v]$ satisfies

$$\max_{u^* \in \Gamma_\delta[B_\sigma(\delta)]} J(u^*) \leq J(u) + \frac{\sigma}{3}. \tag{3.44}$$

At this stage, if we find an element $w \in B_\sigma(\delta)$ such that $J(u) \leq J^\delta(w) + \frac{\sigma}{3}$ then we complete the proof of the lemma. In fact, from (3.35), (3.43) and (3.44),

$$\begin{aligned} c_k &\leq J(u) + \frac{\sigma}{3} \leq J^\delta(w) + \frac{2\sigma}{3} \\ &\leq \max_{w \in B_\sigma(\delta)} J^\delta(w) + \frac{2\sigma}{3} \leq c_k^\delta + \sigma. \end{aligned} \tag{3.45}$$

To finish then, let us find such a w. Choosing $\delta \in (0, \delta_2)$ small enough, for $u = \Gamma_\delta[v]$ we have

$$\begin{aligned} J(u) &= \frac{1}{2} ||v \circ \psi_\delta||^{-1}_{L^{p+1}(\Omega)} \int_\Omega \sum_{i=1}^N \sum_{j=1}^N |g_{i,j}|^2 \\ &\leq \frac{1}{2}(1+\eta)^{1/(p+1)} \int_\Omega \sum_{i=1}^N \sum_{j=1}^N [\delta_{i,j} + O(\delta)]^2 \, |D_j v(\psi_\delta(x))|^2 \\ &\leq (1+\eta)^{1/(p+1)}[1+O(\delta)]^2 \int_\Omega \sum_{j=1}^N |D_j v(\psi_\delta(x))|^2 \, \frac{\det D\psi_\delta(x)}{(1-\eta)} \\ &\leq (1+\eta)^{1/(p+1)} \frac{[1+O(\delta)]^2}{(1-\eta)} J^\delta(v). \end{aligned} \tag{3.46}$$

We see that we can choose $w = v$. Here we used (3.36), (3.37) and the fact that $||v||_{L^{p+1}(\Omega^\delta)} = 1$. □

Proof of Theorem 3.3. Let $\sigma > 0$ small. Considering Lemma 3.4, we choose a $\delta \in (0, \delta_{\sigma/2})$; then, from Lemma 3.2, there exists a $\varepsilon_\delta > 0$ (implicitly depending on σ) such that $c_k \leq c_k^\delta + \sigma/2 \leq c_{k,\varepsilon} + \sigma$, for every $\varepsilon \in (0, \varepsilon_\delta)$. Because of Lemma 3.1, we conclude since $\sigma > 0$ is arbitrary. □

3.4. Asymptotic profiles and concentration phenomena (*Concentración y perfiles asintóticos*)

In this section we study the asymptotic behavior of the solutions, both inside Ω and outside Ω. Throughout this section we use the notation introduced in Section 3.2.

Lemma 3.5. *For every $k \in \mathbb{N}$, as $\varepsilon \to 0$, $w_{k,\varepsilon}$ sub-converges weakly to a $u_k \in \mathrm{H}^1(\Omega)$ such that its restriction to Ω is a solution of (P), with $J(\hat{u}_k|_\Omega) = c_k$, for $\hat{u}_k = (2c_k)^{1/(1-p)} u_k$.*

Proof. First, we prove that for ε_δ small we have that

$$||\hat{w}_{k,\varepsilon}||_{H^1(\mathbb{R}^d)} \leq K_1, \quad \forall \varepsilon \in (0, \varepsilon_\delta), \tag{3.47}$$

where $K_1 > 0$ is a constant, depending only on k. From Lemma 3.1, we get

$$||\nabla \hat{w}_{k,\varepsilon}||^2_{L^2(\mathbb{R}^d)} \leq 2c_k, \quad \forall \varepsilon \in (0, \varepsilon_\delta), \tag{3.48}$$

that is

$$\int_{\mathbb{R}^N} |\nabla \hat{w}_{k,\varepsilon}|^2 \leq \int_{\mathbb{R}^N} |\nabla \hat{w}_k|^2, \tag{3.49}$$

and then, as a consequence of Gagliardo-Nirenberg inequality,

$$||\hat{w}_{k,\varepsilon}||_{L^{2^*}(\mathbb{R}^d)} \leq C c_k^{1/2}, \tag{3.50}$$

for some constant C only depending on N. Given $R \geq 1$, we have

$$\begin{aligned} ||\hat{w}_{k,\varepsilon}||^2_{L^2(\mathbb{R}^d)} &= ||\hat{w}_{k,\varepsilon}||^2_{L^2(\mathbb{R}^d \setminus \Omega^R)} + ||\hat{w}_{k,\varepsilon}||^2_{L^2(\Omega^R)} \\ &\leq \frac{2c_k}{V_R}\varepsilon^2 + ||\hat{w}_{k,\varepsilon}||^2_{L^{2^*}(\Omega^R)} \cdot |\Omega^R|^{2/d} \\ &\leq \frac{2c_k}{V_R} + ||\hat{w}_{k,\varepsilon}||^2_{L^{2^*}(\mathbb{R}^d)} \cdot |\Omega^R|^{2/d}, \end{aligned} \tag{3.51}$$

where we have used the Hölder inequality and the relation

$$||\hat{w}_{k,\varepsilon}||_{L^2(\mathbb{R}^d \setminus \Omega^\delta)} \leq \left(\frac{2c_k}{V_\delta}\right)^{1/2} \varepsilon, \quad \forall \varepsilon \in (0, \varepsilon_\delta), \forall \delta > 0, \tag{3.52}$$

which comes from (3.20). Then, because of (3.48), (3.50) and putting $R = 1$,

$$||\hat{w}_{k,\varepsilon}||^2_{H^1(\mathbb{R}^d)} = ||\nabla \hat{w}_{k,\varepsilon}||^2_{L^2(\mathbb{R}^d)} + ||\hat{w}_{k,\varepsilon}||^2_{L^2(\mathbb{R}^d)} \leq K_1.$$

From the estimate (3.47), there exists a $\hat{u}_k \in \mathrm{H}^1(\Omega)$ such that $\hat{w}_{k,\varepsilon}$ sub-converge weakly and point-wise to $\hat{u}_k \in \mathrm{H}^1(\Omega)$, as $\varepsilon \to 0$.

Now we prove that u_k is solution of (P). Since $\hat{w}_{k,\varepsilon} \in \mathcal{M}_\varepsilon$ is a critical point for J_ε, we have

$$\int_{\mathbb{R}^d} \nabla \hat{w}_{k,\varepsilon} \nabla \phi + \frac{V(x)}{\varepsilon^2} \hat{w}_{k,\varepsilon} \phi = \lambda_{k,\varepsilon} \int_{\mathbb{R}^d} |\hat{w}_{k,\varepsilon}|^{p-1} \hat{w}_{k,\varepsilon} \phi, \quad \forall \phi \in \mathrm{H}^1(\Omega), \tag{3.53}$$

where $\lambda_{k,\varepsilon} = 2c_{k,\varepsilon}$ is the Lagrange multiplier. Then, since

$$\int_{\mathbb{R}^d} \frac{V(x)}{\varepsilon^2} \hat{w}_{k,\varepsilon} \phi = 0, \quad \text{for all} \quad \phi \in \mathrm{C}_0^\infty(\Omega),$$

passing to the limit when $\varepsilon \to 0$, we have

$$\int_\Omega \nabla \hat{u}_k \nabla \phi = \lambda_k \int_\Omega |\hat{u}_k|^{p-1} \hat{u}_k \phi, \quad \forall \phi \in \mathrm{C}_0^\infty(\Omega), \tag{3.54}$$

where $\lambda_k = 2c_k$. Here we have used the fact that $\hat{w}_{k,\varepsilon}$ sub-converge in $\mathrm{L}^{p+1}(\mathbb{R}^d)$ to $\hat{u}_k$, which comes from Lemma 3.1 and the compactness of the embedding $H_\varepsilon \subset \mathrm{L}^{p+1}(\mathbb{R}^d)$.

Considering (3.54) and [9, Prop. IX.18], we are done if we prove that

$$\hat{u}_k(x) = 0, \quad a.e.\, \mathbb{R}^d \setminus \Omega. \tag{3.55}$$

In fact, it would hold $\hat{u}_k|_\Omega \in \mathrm{H}_0^1(\Omega)$, and from (3.54), $J(\hat{u}_k|_\Omega) = c_k$.

Let us prove (3.55). We associate to each $\delta > 0$,

$$\varepsilon_\delta^* = \text{mín}\{\varepsilon_\delta, \frac{V_\delta}{(2c_k)^{1/2}}\}. \tag{3.56}$$

For every $(\delta, \alpha) \in \mathbb{R}_*^+ \times \mathbb{R}_*^+$ we write

$$S_{\delta,\alpha} = \{x \in \mathbb{R}^d \setminus \Omega^\delta : \ |\hat{u}_k(x)| \geq \alpha\}.$$

Let us assume that there exist δ_*, α_*, $\eta > 0$ such that $|S_{\delta_*,\alpha_*}| \geq \eta > 0$. Then, since $S_{\delta_*,\alpha_*} \subset S_{\delta,\alpha_*}$, for all $\delta \in (0, \delta_*)$ we have

$$|S_{\delta,\alpha_*}| \geq \eta > 0, \quad \forall \delta \in (0, \delta_*). \tag{3.57}$$

Considering (V3), we obtain $\delta' \in (0, \delta_*)$ such that

$$V_\delta < \frac{\alpha_*^2 \eta}{2}, \quad \forall \delta \in (0, \delta'). \tag{3.58}$$

Let $\delta_0 \in (0, \delta')$ fixed, then we have that

$$\int_{S_{\delta_0,\alpha*}} |\hat{u}_k|^2 \geq \alpha_*^2 \eta. \tag{3.59}$$

On the other hand, for every $\sigma > 0$ there exists a $\varepsilon_\sigma \in (0, \varepsilon_\delta^*)$ such that

$$||\hat{u}_k||^2_{L^2(S_{\delta_0,\alpha*})} \leq ||\hat{w}_{k,\varepsilon}||^2_{L^2(S_{\delta_0,\alpha*})} + \sigma, \quad \forall \varepsilon \in (0, \varepsilon_\sigma).$$

Thus, for $\sigma = \frac{\alpha_*^2 \eta}{3}$ and $\varepsilon \in (0, \varepsilon_\sigma[$, using (3.52), (3.56) and (3.58), we get

$$\begin{aligned} \int_{S_{\delta_0,\alpha*}} |\hat{u}_k|^2 &\leq \sigma + \int_{S_{\delta_0,\alpha*}} |w_{k,\varepsilon}|^2 \\ &\leq \frac{\alpha_*^2 \eta}{3} + (\frac{2c_k}{V_\delta})\varepsilon^2 \\ &< \frac{\alpha_*^2 \eta}{3} + V_\delta < \frac{5}{6}\alpha_* \eta, \end{aligned} \tag{3.60}$$

which contradicts (3.59). Hence, $|S_{\delta,\alpha}| = 0$, for all $(\alpha, \delta) \in \mathbb{R}_*^+ \times \mathbb{R}_*^+$, that is, we proved (3.55). □

Actually we have strong convergence as the following lemma asserts.

Lemma 3.6. *For every $k \in \mathbb{N}$, as $\varepsilon \to 0$, $w_{k,\varepsilon}$ sub-convergence in the norm of* $\mathrm{H}^1(\Omega)$ *to u_k.*

Proof. From the compactness of the embedding $H_\varepsilon \subset \mathrm{L}^2(\mathbb{R}^d)$, it follows that $\hat{w}_{k,\varepsilon}$ sub-converge in $\mathrm{L}^2(\mathbb{R}^d)$ to $\hat{u}_k$ as $\varepsilon \to 0$; so

$$\lim_{\varepsilon \to 0} \int_{\mathbb{R}^d} |\hat{w}_{k,\varepsilon}|^2 = \int_\Omega |\hat{u}_k|^2.$$

This and (3.49) let us show that

$$\limsup_{\varepsilon \to 0} ||\hat{w}_{k,\varepsilon}||_{H^1(\mathbb{R}^d)} \leq ||\hat{u}_k||_{H^1(\mathbb{R}^d)},$$

concluding the proof. □

Our next goal is to obtain an exponential control of the decay of the family $\{w_{k,\varepsilon}\}$ outside Ω. For this purpose we obtain a general L^∞ estimate for solutions of an elliptic inequality, following the Moser iteration technique. We have

Proposition 3.1. *Let $D \subset \mathbb{R}^d$ be open and connected. If w is a classical solution of the elliptic inequality*

$$\begin{cases} \Delta w - f(w) \geq 0 & \text{in} \quad D, \\ \quad w > 0 & \text{in} \quad D, \\ \quad w = 0 & \text{on} \quad \partial D, \end{cases} \tag{3.61}$$

where $N \geq 3$, $p+1 \in (2, 2^*)$ and f satisfies

$$tf(t) \leq ct^{p+1}, \quad \forall t \in \mathbb{R}^+, \tag{3.62}$$

for some constant $c > 0$. If moreover $w \in \mathrm{H}_0^1(D)$ then there exists a constant $C = C(c, p, N) > 0$ such that

$$||w||_{L^\infty(D)} \leq C\, ||w||_{L^{2^*}(D)}^{4/[(N+2)-p(N-2)]}. \tag{3.63}$$

This result was proved in [10] assuming that $D \subset \mathbb{R}^d$ is smooth and bounded. It can be extended to a non-necessarily bounded D nor regular ∂D. We can follow the step in [10], by choosing a slightly modified test depending on a parameter, in order to avoid the possible non-regularity of the boundary. We omit the details.

Lemma 3.7. *For every $k \in \mathbb{N}$ there exists a $K_2 > 0$ such that*

$$||w_{k,\varepsilon}||_{L^\infty(\mathbb{R}^d)} < K_2, \quad \forall \varepsilon \in (0, \varepsilon_\delta). \tag{3.64}$$

Proof. Given $\varepsilon \in (0, \varepsilon_\delta)$, we consider D_ε^+ a connected component of the set $\{x \in \mathbb{R}^d : \; w_{k,\varepsilon} > 0\}$. So, we have

$$\begin{cases} \Delta w_{k,\varepsilon} + w_{k,\varepsilon}^p \geq 0 & \text{in} \quad D_\varepsilon^+, \\ \quad w_{k,\varepsilon} > 0 & \text{in} \quad D_\varepsilon^+, \\ \quad w_{k,\varepsilon} = 0 & \text{on} \quad \partial D_\varepsilon^+, \end{cases} \tag{3.65}$$

hence, from (3.50) and Proposition 3.1,

$$||w_{k,\varepsilon}||_{L^\infty(D_\varepsilon^+)} \leq K_2, \quad \forall \varepsilon \in (0, \varepsilon_\delta), \tag{3.66}$$

where the constant K_2 depends on d, k and p. Since D_ε^+ is arbitrary, the inequality holds in $\{x \in \mathbb{R}^d : \; w_{k,\varepsilon} > 0\}$. By a similar argument we also show that the inequality holds in $\{x \in \mathbb{R}^d : \; w_{k,\varepsilon} < 0\}$. □

Remark 3.9. Since $v_{k,\varepsilon} = \varepsilon^{2/(p-1)} w_{k,\varepsilon}$, it follows from Lemma 3.7 that

$$\lim_{\varepsilon \to 0} ||v_{k,\varepsilon}||_{L^\infty(\mathbb{R}^d)} = 0, \quad \forall k \in \mathbb{N}. \tag{3.67}$$

Moreover, since $||u_k||_{L^{p+1}(\mathbb{R}^d)} \neq 0$ for all $k \in \mathbb{N}$, it is clear that there exists a constant $\eta_k > 0$ such that

$$\liminf_{\varepsilon \to 0} \frac{||v_{k,\varepsilon}||_{L^\infty(\mathbb{R}^d)}}{\varepsilon^{2/(p-1)}} \geq \eta_k > 0. \tag{3.68}$$

In order to obtain the exponential decay of $w_{k,\varepsilon}$, we shall give a comparison argument as in [11]. We consider a positive solution for the problem

$$\begin{cases} \Delta U - 2bU = 0 & \text{in} \quad \mathbb{R}^d \setminus \Omega^\delta, \\ U = a & \text{on} \quad \partial\Omega^\delta, \\ \lim_{|x|\to\infty} U(x) = 0, \end{cases} \tag{3.69}$$

where $a, b > 0$. Such a solution satisfies

$$U(x) \leq C \exp\{-b \cdot \operatorname{dist}(x, \Omega^\delta)\}, \quad \forall x \in \mathbb{R}^d \setminus \Omega^\delta. \tag{3.70}$$

for some constant C depending on a and Ω^δ, see [11, Lemma 2.7].

<u>Lemma</u> 3.8. *For every $k \in \mathbb{N}$, $\delta, c > 0$, there exists $\varepsilon_{**} \in (0, \varepsilon_\delta)$ such that*

$$|w_{k,\varepsilon}(x)| < C \cdot \exp\{-\frac{c}{\varepsilon} \cdot \operatorname{dist}(x, \Omega^\delta)\}, \quad \forall x \in \mathbb{R}^d, \forall \varepsilon \in (0, \varepsilon_{**}), \tag{3.71}$$

where C depends on K_2 and Ω^δ.

Proof. Let $\varepsilon_* \in (0, \varepsilon_\delta)$ such that $V_\delta > (K_2 + 2c/\varepsilon_*)\varepsilon_*^2$. Then, from Lemma 3.7 and for all $\varepsilon \in (0, \varepsilon_*)$ and $x \in \mathbb{R}^d \setminus \overline{\Omega^\delta}$, we have that

$$F_{k,\varepsilon}(x) \equiv \frac{V(x)}{\varepsilon^2} - |w_{k,\varepsilon}|^{p-1} \geq \frac{V_\delta}{\varepsilon^2} - K_2 > 2\frac{c}{\varepsilon}.$$

Now we consider U a solution to problem (3.69) with $a = K_2$ and $b = c/\varepsilon$. Then,

$$\begin{cases} \Delta U - F_{k,\varepsilon}(x)U \quad \leq 0 & \text{in} \quad \mathbb{R}^d \setminus \Omega^\delta, \\ \qquad\qquad U \quad = K_2 & \text{on} \quad \partial\Omega^\delta, \\ \lim_{|x|\to\infty} U(x) = 0, \end{cases} \tag{3.72}$$

from where it follows that

$$\begin{cases} \Delta(U - w_{k,\varepsilon}) - F_{k,\varepsilon}(x)(U - w_{k,\varepsilon}) \leq 0 & \text{in} \quad \mathbb{R}^d \setminus \Omega^\delta, \\ U - w_{k,\varepsilon} > 0 & \text{on} \quad \partial\Omega^\delta, \\ \text{lím}_{|x|\to\infty}(U(x) - w_{k,\varepsilon}(x)) = 0. \end{cases} \tag{3.73}$$

Now it is clear that

$$w_{k,\varepsilon}(x) \leq U(x), \quad \forall x \in \mathbb{R}^d \setminus \Omega^\delta.$$

Analogously we can prove that

$$-U(x) \leq w_{k,\varepsilon}(x), \quad \forall x \in \mathbb{R}^d \setminus \Omega^\delta.$$

Then, using (3.70) we obtain

$$|w_{k,\varepsilon}(x)| \leq C \exp\{-\frac{c}{\varepsilon}\text{dist}(x, \Omega^\delta)\}, \quad \forall x \in \mathbb{R}^d \setminus \Omega^\delta,$$

and, enlarging C if necessary, we finally get the inequality in all $\mathbb{R}^d$. □

3.5. Asymptotic behavior at the boundary (*Comportamiento asintótico sobre la frontera*)

We already know that the sequence $w_{k,\varepsilon}$ converges in $H^1(\mathbb{R})$ to a function u which is a solution of (P) in Ω. By elliptic regularity it is not hard to prove that on each compact set $D \subset \Omega$, the convergence of $w_{k,\varepsilon}$ to u is uniform on D. On the other hand, outside Ω, namely in Ω^δ, we have exponential decay according to Lemma 3.8. The uniform behavior of $w_{k,\varepsilon}$ on the boundary of Ω is not covered by these two arguments. In this section we prove

Proposition 3.2. *The family of solutions $w_{k,\varepsilon}$ verifies*

$$\lim_{\varepsilon\to 0} \max_{x\in\partial\Omega} |w_{k,\varepsilon}(x)| = 0, \quad \forall k \in \mathbb{N}. \tag{3.74}$$

For proving this proposition we see two preliminary lemmas. Let $\delta > 0$ be small enough so that the set $\Omega_\delta \equiv \{x \in \Omega : \text{dist}(x, \partial\Omega) > \delta\}$ is not empty. We define the ring around $\partial\Omega$ as $R(\delta) = \Omega^\delta \setminus \overline{\Omega_\delta}$ and we consider $M_\varepsilon(\delta) = \text{máx}_{x\in\partial R(\delta)} |w_{k,\varepsilon}(x)|$ for $k \in \mathbb{N}$ fixed. First we show that

Lemma 3.9. *Given $\sigma > 0$, there exists $\delta_\sigma > 0$ such that*

$$\max_{x\in R(\delta)} |w_{k,\varepsilon}(x)| \leq M_\varepsilon(\delta) + \sigma, \quad \forall \delta \in (0, \delta_\sigma). \tag{3.75}$$

Proof. For notational convenience we denote $w = w_{k,\varepsilon}$ and $R^{\pm}(\delta) = \{x \in R(\delta) : \pm w > 0\}$. Then we have

$$\begin{cases} \pm\Delta w \pm |w|^{p-1}w \geq 0, & \text{in} \quad R^{\pm}(\delta); \\ \pm w \geq 0, & \text{on} \quad \partial R^{\pm}(\delta) \end{cases} \tag{$D^{\pm}$}$$

We consider only (D^+) since the other case is analogous. We put $v = w - M_\varepsilon(\delta)$ to get

$$\begin{cases} \Delta v \geq f, & \text{in} \quad R^{+}(\delta); \\ v \leq 0, & \text{on} \quad \partial R^{+}(\delta) \end{cases} \tag{3.76}$$

where $f \equiv -|w|^{p-1}(M_\varepsilon(\delta) + v)$. Then, using the Alexandroff Maximum Principle ([48, Th.2.21]), we obtain

$$\begin{aligned} \sup_{R^+(\delta)} v &\leq C \cdot ||f^-||_{L^N(R^+(\delta))} \\ &\leq C|R^+(\delta)|^{1/N} K_2^{p-1}(M_\varepsilon(\delta) + \sup_{R^+(\delta)} v), \end{aligned}$$

where $C = C(N, \mathrm{diam}(\Omega)) > 0$. Now choosing $\delta_\sigma > 0$ small enough, we get

$$\sup_{R^+(\delta)} w \leq M_\varepsilon(\delta) + \sigma, \quad \forall \delta \in (0, \delta_\sigma). \tag{3.77}$$

In a similar way, decreasing δ_σ if necessary, we find also

$$\inf_{R^-(\delta)} w \geq -M_\varepsilon(\delta) - \sigma, \quad \forall \delta \in (0, \delta_\sigma), \tag{3.78}$$

completing the proof of the lemma. □

Next we control the values of w on $\partial R(\delta)$, that is

Lema 3.1. *Given $\sigma > 0$, there exist $\delta', \varepsilon' > 0$ such that*

$$M_\varepsilon(\delta') < \sigma, \quad \forall \varepsilon \in (0, \varepsilon'). \tag{3.79}$$

We observe that with this lemma and Lemma 3.9 we can complete the proof of Proposition 3.2. In fact $\partial\Omega \subset R(\delta)$ and so $\max_{x\in\partial\Omega}|w_{k,\varepsilon}(x)| \leq \max_{x\in R(\delta)}|w_{k,\varepsilon}(x)|$.

Proof of lemma 3.1. Denoting

$$m_\delta(\varepsilon) = \max_{x\in\partial\Omega_\delta}|w_{k,\varepsilon}(x)| \quad \text{and} \quad m^\delta(\varepsilon) = \max_{x\in\partial\Omega^\delta}|w_{k,\varepsilon}(x)|,$$

we see that we need to show that $m_\delta(\varepsilon)$ and $m^\delta(\varepsilon)$ are controlled by σ.

First, we see that

$$\lim_{\varepsilon\longrightarrow 0} m^\delta(\varepsilon) = 0.$$

In fact, outside $\Omega^{\delta/2}$, $w_{k,\varepsilon}$ decay exponentially, as proved in Lemma 3.8 then $w_{k,\varepsilon} \to 0$ uniformly in $\partial\Omega^\delta$.

Second, we study $m_\delta(\varepsilon)$. We denote by K_{c_k} the set of critical points of the functional J corresponding to the critical value c_k. According to Lemmas 3.5 and 3.6, there exists $u \in K_{c_k}$ and a sequence $\{\varepsilon_i\}_{i\in\mathbb{N}}$ such that $\lim_{n\to\infty}\varepsilon_n = 0$ and $w_{k,\varepsilon_n} \equiv w_n \to u$ in $\mathrm{H}^1(\Omega)$ and point-wise. We choose $\eta > 0$ such that $R_\delta(\eta) = \Omega_{\delta-\eta} \setminus \overline{\Omega_{\delta+\eta}}$ verifies $R_\delta(\eta) \cap \partial\Omega = \emptyset$. From elliptic estimates, we see that for each compact set $D \subset \Omega$, the convergence of w_n to u is uniform in D. Then, in particular, given $\sigma > 0$, there exists a $n^* = n^*(\sigma, w) \in \mathbb{N}$ such that

$$\max_{x\in\overline{R_\delta(\eta)}}|w_n(x) - u(x)| < \frac{\sigma}{2}, \quad \forall n > n^*. \tag{3.80}$$

On other hand, since $u|_{\mathbb{R}^d\setminus\overline{\Omega}} = 0$ and u is a solution of (P), there exists a $\delta' = \delta'(\sigma, w) > 0$ such that

$$\max_{x\in\overline{R_{\delta'}(\eta)}}|u(x)| < \frac{\sigma}{2}. \tag{3.81}$$

Then, from (3.80) and (3.81), we get

$$m_{\delta'}(\varepsilon_n) < \sigma, \quad \forall n > n^*. \tag{3.82}$$

We see that the value n^* and δ' may depend on u. However, one can argue using the compactness of the set K_{c_k}, that they can be chosen so they actually depend only on k, but not on the particular $u \in K_{c_k}$. □

Capítulo 4

Propiedades de compacidad para operadores de traza y aplicaciones a la Mecánica Cuántica

Como se dijo en la Presentación, mantenemos el idioma en que será publicado el artículo [27]. Los comentarios adicionales serán provistos en notas al pie. La Sección 4.5 no aparece en [27]; la presentamos pues corresponde a una aplicación directa del material que le precede.

Abstract (*Resumen*)

Interpolation inequalities of Gagliardo-Nirenberg type and compactness results for self-adjoint finite-trace operators with finite kinetic energy are established. Applying these results to the minimization of free energy functionals which are not necessarily convex, we characterize for instance stationary states of the Hartree problem with temperature. Equivalent results in the mixed states representation for quantum mechanics also hold.

4.1. Introduction (*Introducción*)

The first eigenvalue $\lambda_{V,1}$ of a Schrödinger operator $-\Delta + V$ can be estimated using Sobolev's inequalities, [72, 68, 42]. In some recent papers, [7, 73, 26], a precise connection has been given between the optimal estimates of $\lambda_{V,1}$ in terms of a norm of V and the optimal constants in some related Gagliardo-Nirenberg inequalities. Such inequalities admit optimal functions, see [76, 26].

In the case of orthonormal and sub-orthonormal systems, interpolation inequalities of Gagliardo-Nirenberg type provide informations on optimal constants in inequalities, see [57, 56, 40, 32], which can be extended to Lieb-Thirring type inequalities, [55]. We refer to [26] for references in this direction and precise statements concerning the relation between optimal constants in these two families of inequalities, in the case of the euclidean space $\mathbb{R}^d$.

Conversely, the knowledge of Lieb-Thirring inequalities can be rephrased into interpolation inequalities for *mixed states,* which are infinite systems of orthogonal functions with occupations numbers, see [26]. It is well known that an equivalent formulation holds in terms of operators. In this paper we rewrite and extend these interpolation inequalities for *trace-class self-adjoint operators* and focus on the case of a domain $\Omega \subset \mathbb{R}^d$. We also study, at the level of the operators, the *compactness properties* of the corresponding embeddings, which extend the well known properties of Sobolev's embeddings to trace-class self-adjoint operators.

An important source of motivation is the paper by P. Markowich, G. Rein and G. Wolansky, [60], which was devoted to the analysis of the stability of the Schrödinger-Poisson system. It involves in a crucial way some functionals which are a key tools of our approach, and that we will call *free energy functionals* because of their interpretation in physics. In [60], the authors refer to such functionals as *Casimir* functionals, for historical reasons in mechanics, [77]. During the last few years, various results based on free energy functionals, which are sometimes also called *generalized entropy functionals,* have been achieved in the theory of partial differential equations. We can for instance quote nonlinear stability results for fluid and kinetic equations, see for instance [77, 44, 45, 67], studies of the qualitative behavior of the solutions of kinetic and diffusion equations, including large time asymptotics and diffusion limits, see, *e.g.,* [6, 14, 29], and applications to free boundary problems: [30], or quantum mechanics: [59, 60]. At a formal level, these various functionals are all more or less the same object. The precise connection is still being studied at the moment from a mathematical point of view, although the correspondence at a physical level makes no more doubts.

Minimizing the free energy functional for a given potential is equivalent to proving Lieb-Thirring inequalities, while the optimization on the potential provides interpolation inequalities. Such questions have been only tangentially studied in [60], since in this paper the potential is given by an electrostatic Poisson law with homogeneous Dirichlet boundary conditions and therefore always positive. Here we work in a much more general setting, which physically could correspond to external potentials with a singularity (for instance created by doping charge impurities in a semi-conductor) and our first task is therefore to bound from below the free energy functional, *i.e.* to establish adapted Lieb-Thirring inequalities. Our second step consists in reformulating these inequalities in terms of Gagliardo-Nirenberg type interpolation inequalities for operators, and to study the compactness properties of the corresponding embeddings. Afterwards, the minimization procedure becomes more or less trivial, thus giving for almost no work the existence of minimizers, including in the case of non-linear models involving, for instance, a Poisson coupling.

Let Ω be a domain in $\mathbb{R}^d$ with smooth boundary and consider a smooth positive potential V on $\overline{\Omega}$. As a starting point, we are interested in inequalities of Lieb-Thirring type for the Schrödinger operator $-\Delta + V$. Let $\{\lambda_{V,i}\}_{i\in\mathbb{N}}$ be the corresponding unbounded non-decreasing sequence of eigenvalues. As a straightforward consequence of the results of [26], the following inequality holds: for any $\gamma > d/2$, there exists some explicit constant $C(\gamma)$, which does not depend on V, such that

$$\sum_{i\in\mathbb{N}} \left(\lambda_{V,i}\right)^{-\gamma} \leq C(\gamma) \int_\Omega V^{d/2-\gamma}\, dx \,, \tag{4.1}$$

(see Example 1 in Section 4.3.1 for a precise statement). This inequality arises as a special case of a master inequality which goes as follows. Consider a sequence of orthonormal functions $\{\psi_i\}_{i\in\mathbb{N}}$ and a sequence $\{\nu_i\}_{i\in\mathbb{N}}$ of non-negative real numbers. The sequence $\{(\nu_i, \psi_i)\}_{i\in\mathbb{N}} \in \ell^1 \times \mathrm{L}^2(\Omega)$ is called a *mixed state* in the physics literature. The *master inequality* is

$$\begin{aligned} \sum_{i\in\mathbb{N}} \beta(\nu_i) + \frac{1}{2} \sum_{i\in\mathbb{N}} \nu_i \left(\psi_i, (-\Delta + V)\, \psi_i\right)_{L^2(\Omega)} &\geq - \sum_{i\in\mathbb{N}} F\left(\lambda_{V,i}\right) \\ &\geq - \int_\Omega G(V)\, dx \,. \end{aligned} \tag{4.2}$$

Then (4.1) corresponds to the case $\beta_m(\nu) = -c_m\, \nu^m$ for some explicit constant c_m, $m = \gamma/(\gamma+1) \in (d/(d+2), 1)$, $F(s) \equiv s^{-\gamma}$ and $G(s) \equiv C(\gamma)\, s^{d/2-\gamma}$.

The important point is that Inequality (4.2) then holds for any potential and any mixed state. Other choices can also be done, for instance $\beta_1(s) \equiv s\log s - s$, $F(s) \equiv e^{-s}$ and $G(s) \equiv (4\pi)^{-d/2}\,e^{-s}$, thus showing the following Lieb-Thirring type inequality

$$\sum_{i\in\mathbb{N}} e^{-\lambda_{V,i}} \leq (4\pi)^{-d/2}\int_\Omega e^{-V}\,dx\;.$$

Using the Hilbert-Schmidt theorem, by considering self-adjoint trace-class operators L with kernel $K_L(x,y) \equiv \sum_{i\in\mathbb{N}} \nu_i\,\psi_i(x)\,\psi_i(y)$, we can reformulate the first part of Inequality (4.2) in terms of operators, and get

$$\mathrm{Tr}\,[\beta(L) + (-\Delta + V - \lambda)\,L] \geq -\mathrm{Tr}\,\big[F\big(-\Delta + V - \lambda\big)\big]$$

for some parameter λ that we take equal to 0 for the moment. Up to now, V was assumed to be positive. Our first main result is an extension of Inequality (4.2) to potentials which may change sign. For a non-negative perturbation W of a sign changing potential V, Inequality (4.2) is replaced by

$$\mathrm{Tr}\,[\beta(L) + (-\Delta + V + W - \lambda)\,L] \geq -\,\varepsilon^{-d/2}\int_\Omega G(W)\,dx\;, \tag{4.3}$$

for some ε and λ to be fixed later. An optimization on W then gives an interpolation inequality of Gagliardo-Nirenberg type. To give a precise statement, let us fix some notations. Consider a non-negative function f satisfying $\int_0^\infty f(t)\,\big(1+t^{-d/2}\big)\,t^{-1}\,dt < \infty$, define

$$F(s) := \int_0^\infty e^{-t\,s}\,f(t)\,\frac{dt}{t} \quad\text{and}\quad G(s) := \int_0^\infty e^{-t\,s}\,(4\pi\,t)^{-d/2}\,f(t)\,\frac{dt}{t}\;,$$

and let β and τ be such that $\beta(s) \equiv F^*(-s)$ and $G(s) \equiv \tau^*(-s)$. Here F^* denotes the Legendre-Fenchel transform of F. We also use the notation ρ_L for the non-negative function $\sum_{i\in\mathbb{N}} \nu_i\,|\psi_i|^2 \in L^1(\Omega)$, using a mixed state representation $\{(\nu_i,\psi_i)\}_{i\in\mathbb{N}}$ associated to L. Some standard precautions are needed to identify $\rho_L(x)$ with $K_L(x,x)$.

Theorem 4.1. *For a given potential V, assume that for some $\varepsilon \in (0,1)$, $-(1-\varepsilon)\,\Delta + V$ is bounded from below by some constant λ, in the sense of operators. With the above notations, Inequality (4.3) holds for any non-negative self-adjoint trace-class operator L, and moreover*

$$\mathrm{Tr}\,[\beta(L) + (-\Delta + V - \lambda)L] \geq \varepsilon^{-\frac{d}{2}}\int_\Omega \tau\left(\varepsilon^{\frac{d}{2}}\,\rho_L(x)\right)\,dx\;.$$

The core of the proof is based on a minimization with respect to the mixed state $\{(\nu_i, \psi_i)\}_{i\in\mathbb{N}}$, which in the end requires that ψ_i is an eigenfunction of $-\Delta + V$ and $\nu_i = (\beta')^{-1}(\lambda - \lambda_{V,i})$. Since the domain Ω is bounded, at least when $V \equiv 0$ and $\lambda = 0$, these inequalities can even be slightly improved, but the improvement on the constant depends on Ω and the above inequality as well as Inequality (4.3) are optimal if one looks for constants which are independent of Ω.

In the two interesting cases $F(s) \equiv s^{-\gamma}$ and $F(s) \equiv e^{-s}$, we obtain the following interpolation inequalities

$$\mathrm{Tr}\,[-\Delta L] + \kappa(\gamma) \int_\Omega \rho_L^q \, dx \geq c_m \,\mathrm{Tr}\,[L^m] \ ,$$

where $q \equiv (2\gamma - d)/(2(\gamma+1) - d) \in (0,1)$ and $\kappa(\gamma)$ is an explicit positive constant, and

$$\int_\Omega \rho_L \log \rho_L \, dx \leq \mathrm{Tr}\,[L \, \log L] + \frac{d}{2} \log\left(\frac{e}{2\pi d} \, \frac{\mathrm{Tr}\,[-\Delta L]}{\|L\|_1}\right) \|L\|_1 \ ,$$

where L is any non-negative self-adjoint trace-class operator. For simplicity, the inequalities written here correspond to the case where V is non-negative, but more general statements corresponding to a sign changing potential V can be deduced from Theorem 4.1. See Theorem 4.3 and Corollaries 4.1, 4.3, 4.4, 4.5 for various improvements.

The interpolation inequalities of Theorem 4.1 generalize for self-adjoint trace-class operators the usual Gagliardo-Nirenberg inequalities. Exactly as for the embedding $\mathrm{H}^1_0(\Omega) \hookrightarrow \mathrm{L}^2(\Omega)$, some compactness can be expected. Such a statement constitutes our second main result.

Theorem 4.2. *Under the assumptions of Theorem 4.1, if $\{L_n\}_{n\in\mathbb{N}^*}$ is a sequence of non-negative self-adjoint trace-class operators, with bounded trace such that*

$$\{\mathrm{Tr}\,[\beta(L_n) + (-\Delta + V - \lambda)\, L_n]\}_{n\in\mathbb{N}^*}$$

is bounded, then $\{L_n\}_{n\in\mathbb{N}^*}$ is relatively compact and converges to some non-negative self-adjoint compact operator L up to the extraction of a subsequence. Morover, ρ_{L_n} converges to ρ_L in $L^q(\Omega)$, for any $q \in [1,\infty]$ if $d = 1$, $q \in [1,\infty)$ if $d = 2$ and $q \in [1, d/(d-2)]$ if $d \geq 3$.

This paper is organized as follows. Section 4.2 is devoted to definitions, preliminary results and consequences of the results of [26]. In Section 4.2.2 we introduce a set of trace-class operators having the form $F(-\Delta)$. To this class belong the operators generated by the Boltzmann distribution and the Fermi-Dirac statistics, see Example 3 in Section 4.2.2. The space $\mathcal{S}_1$ of *trace-class self-adjoint operators*, which are also known as *nuclear self-adjoint operators*, plays the role of the space L^1 and the spaces $\mathcal{S}_q$ can be felt as the spaces L^q, $q \in [1, \infty]$. Inspired by this analogy, we define in Section 4.2.3 the Sobolev-like cones $\mathcal{W}^{l,p}$ as appropriate subsets of $\mathcal{S}_1$. As far as we know the definition of these cones is a novelty. Basic properties (Proposition 4.1) of these cones and a regularity result (Proposition 4.2) concerning the density functions associated to $\mathcal{H}^1 = \mathcal{W}^{1,2}$ are established in Section 4.2.3. The *free energy functional*

$$\mathcal{F}^{\lambda}_{V,\beta}(L) \equiv \mathrm{Tr}\,[\beta(L) + (-\Delta + V - \lambda)L]$$

is defined in Section 4.2.4.

Theorems 4.1 and 4.2 are proved in Section 4.3. An improved interpolation inequality is given in Theorem 4.3. The key estimate is a convexity inequality (Lemma 4.1) which allows simultaneously to minimize the *free energy functional* and to get some coercivity even if V changes sign (Proposition 4.5). The compactness result then follows (see Theorem 4.4 for a detailed statement and Corollary 4.7 for an extension).

As a simple consequence, in Section 4.4, we prove the existence of minimizers in several cases of interest in quantum mechanics. Some additional references for applications in quantum mechanics are given at the end of this paper.

4.2. Definitions and preliminary results (*Definiciones y resultados preliminares*)

4.2.1. The operators setting (*El universo de operadores*)

Let Ω be a domain in $\mathbb{R}^d$, $d \in \mathbb{N}^*$. We assume that $\partial\Omega$ is of class C^1. We will denote respectively by $\mathcal{L}(\mathrm{L}^2(\Omega))$, $\mathcal{I}_\infty$ and $\mathcal{S}_\infty$ the spaces of bounded linear, compact and compact self-adjoint operators acting on $\mathrm{L}^2(\Omega)$, and by

$\| \cdot \|$ the standard norm on $\mathcal{L}(\mathrm{L}^2(\Omega))$. We also define the spaces

$$\mathcal{I}_2 \equiv \Big\{ L \in \mathcal{I}_\infty \ : \ \big[\operatorname{Tr}(|L|^2) \big]^{1/2} < \infty \Big\} ,$$
$$\mathcal{I}_1 \equiv \Big\{ L \in \mathcal{I}_\infty \ : \ \sum_{i \in \mathbb{N}} \big| (\chi_i,\, L\chi_i)_{\mathrm{L}^2(\Omega)} \big| < \infty \Big\} ,$$

where $\{\chi_i\}_{i\in\mathbb{N}}$ is any complete orthonormal system in $\mathrm{L}^2(\Omega)$. The space $\mathcal{I}_1$ is called the space of *trace class* operators and its elements are indifferently called *trace class* operators or *nuclear operators*. Let $L \in \mathcal{I}_1$ be given. The *trace* of L is the value

$$\operatorname{Tr}[L] \equiv \sum_{i \in \mathbb{N}} (\chi_i,\, L\chi_i)_{\mathrm{L}^2(\Omega)} \ , \tag{4.4}$$

where $\{\chi_i\}_{i\in\mathbb{N}}$ is any complete orthonormal system in $\mathrm{L}^2(\Omega)$. Notice that $\operatorname{Tr}[L]$ does not depend on the choice of $\{\chi_i\}_{i\in\mathbb{N}}$. The space $\mathcal{I}_2$ is the space of the *Hilbert-Schmidt operators*. Equiped with the scalar product $\langle L, R\rangle_2 \equiv \operatorname{Tr}[R^*L]$, $\mathcal{I}_2$ is a Hilbert space. According to, *e.g.*, [64, Theorem VI.23], an operator $L \in \mathcal{L}(\mathrm{L}^2(\Omega))$ is of Hilbert-Schmidt type if and only if there is a function $K_L \in \mathrm{L}^2(\Omega \times \Omega)$, the *kernel of* L, such that

$$\|L\|_2^2 = \iint_{\Omega\times\Omega} |K_L(x,y)|^2 \, dx\, dy$$

is finite and

$$(L\eta)(x) = \int_\Omega K_L(x,y)\, \eta(y)\, dy \quad \text{for a.e. } x \in \Omega \ , \quad \forall\, \eta \in \mathrm{L}^2(\Omega) \ .$$

For $L \in \mathcal{S}_\infty$ we denote by $\{\nu_i(L)\}_{i\in\mathbb{N}}$, or simply $\{\nu_i\}_{i\in\mathbb{N}}$ if there is no confusion, the sequence of eigenvalues counted with multiplicity, which is well defined by the Hilbert-Schmidt theorem. Unless it is explicitly specified $\{\nu_i\}_{i\in\mathbb{N}}$ will be ordered in a way such that $\{|\nu_i(L)|\}_{i\in\mathbb{N}}$ is non-increasing. We adopt the convention that if both ν and $-\nu$ are eigenvalues, $-|\nu|$ comes first. We will denote by $\{\psi_i(L)\}$, or simply $\{\psi_i\}_{i\in\mathbb{N}}$ if there is no ambiguity, an associated orthonormal system of eigenfunctions, which is complete in $\mathrm{L}^2(\Omega)$: see, *e.g.*, [9, Chapter VI]. From now on we are only dealing with self-adjoint operators and consider for any $q \in [1, \infty)$ the spaces

$$\mathcal{S}_q \equiv \Big\{ L \in \mathcal{S}_\infty \ : \ \|L\|_q \equiv \Big(\sum_{i\in\mathbb{N}} |\nu_i|^q \Big)^{1/q} < \infty \Big\} .$$

If $L \in \mathcal{S}_2$, given an orthonormal system of eigenfunctions $\{\psi_i\}_{i\in\mathbb{N}}$ associated to L, K_L is explicitly given by

$$K_L(x,y) = \sum_{i\in\mathbb{N}} \nu_i \, \psi_i(x) \, \overline{\psi}_i(y) \quad \text{for a.e. } x,\, y \in \Omega \, .$$

If $L \in \mathcal{S}_1$, then $\|L\|_1 = \mathrm{Tr}(|L|)$. Let $\{\psi_i\}_{i\in\mathbb{N}}$ be an orthonormal system of eigenfunctions associated to $L \in \mathcal{S}_1$. The function given by

$$\rho_L(x) \equiv \sum_{i\in\mathbb{N}} \nu_i \, |\psi_i(x)|^2, \quad x \in \Omega \; a.e. \, ,$$

is in $\mathrm{L}^1(\Omega)$. Notice again that ρ_L does not depend on the special choice of $\{\psi_i\}_{i\in\mathbb{N}}$. We have that

$$\int_\Omega |\rho_L(x)| \, dx \le \|L\|_1 = \int_\Omega \rho_{|L|}(x) \, dx \quad \forall \, L \in \mathcal{S}_1 \, .$$

If additionally L is a non-negative operator, ρ_L is also non-negative, it is called the *density function associated to* L and $\|L\|_1 = \mathrm{Tr}\,[L] = \int_\Omega \rho_L(x)\,dx$. Such a definition is consistent with the density operator formalism in quantum mechanics.

In some cases (4.4) makes sense for an operator L which is not in $\mathcal{S}_1$, but is for instance in $\mathcal{L}(\mathrm{L}^2(\Omega))$ and such that the right hand side in (4.4) is finite. We shall then write $\mathrm{tr}\,[L]$ instead of $\mathrm{Tr}\,[L]$.

Let us recall some other well known facts on $\mathcal{S}_q$. See, *e.g.*, [65, Prop. 5-6] for more details. Some of these results also apply to operators which are not self-adjoint, but this is outside of the scope of this paper.

i) $\mathcal{S}_q$ equipped with the norm $\|\cdot\|_q$ is a Banach space and $\|L\| = \lim_{q\longrightarrow\infty} \|L\|_q$, but $\mathcal{S}_q \subsetneq \mathcal{S}_\infty$ for any $q \in [1,\infty)$.

ii) If $1 < q_1 < q_2 < \infty$, then

$$\|L\|_{q_2} \le \|L\|_{q_1} \quad \forall \, L \in \mathcal{S}_{q_1} \, ,$$

so that $\mathcal{S}_1 \subset \mathcal{S}_{q_1} \subset \mathcal{S}_{q_2} \subset \mathcal{S}_\infty$.

iii) $\mathcal{S}_q$ is the closure of the space of finite rank self-adjoint operators with respect to the norm $\|\cdot\|_q$.

iv) If $1 \leq q \leq \infty$ and $q^{-1} + r^{-1} = 1$, then

$$\|A\,B\|_1 \leq \|A\|_q\,\|B\|_r \quad \forall\, A \in \mathcal{S}_q\,,\ B \in \mathcal{S}_r\,. \tag{4.5}$$

In case $q = \infty$ (and $r = 1$), $\|\cdot\|_\infty = \|\cdot\|$, the usual norm of bounded operators.

4.2.2. Operators of the form $\mathbf{F}(-\boldsymbol{\Delta})$ and Casimir-type functions (*Operadores de la forma* $\mathbf{F}(-\boldsymbol{\Delta})$ *y funciones tipo Casimir*)

In the case of a domain $\Omega \subset \mathbb{R}^d$, a useful class of operators can be obtained out of the Laplacian. Let $\{\lambda_{0,i}\}_{i\in\mathbb{N}}$ and $\{\phi_{0,i}\}_{i\in\mathbb{N}}$ be the eigenvalues and the eigenfunctions of the Laplacian in the case of homogeneous Dirichlet boundary conditions. According to [9, Theorem IX.31] for instance, for each $i \in \mathbb{N}$, consider

$$\begin{cases} -\Delta\phi_{0,i} = \lambda_{0,i}\phi_{0,i} & \text{in } \Omega\,, \\ \phi_{0,i} \in \mathrm{H}_0^1(\Omega) \cap \mathrm{C}^\infty(\Omega)\,. \end{cases} \tag{4.6}$$

The ordered sequence $0 < \lambda_{0,1} < \lambda_{0,2} \leq \lambda_{0,3} \leq \ldots$ diverges and $\{\phi_{0,i}\}_{i\in\mathbb{N}}$ is a complete orthonormal system in $\mathrm{L}^2(\Omega)$.

Definition 4.1. We shall say that a function $F : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ is of $\mathcal{C}_{-\Delta,\Omega}$*-class* if it is convex and $\sum_{i\in\mathbb{N}} F(\lambda_{0,i})$ is finite.

The Spectral Theorem (see, *e.g.*, [64, Theorem VIII.5]) then allows to define the nuclear operator $F(-\Delta)$ for each $F \in \mathcal{C}_{-\Delta,\Omega}$. From this definition it also follows that the point spectrum $\sigma_p(-\Delta) \equiv \{\lambda_{0,i} : i \in \mathbb{N}\}$ of $-\Delta$ is contained in the domain $\mathrm{Dom}(F) \equiv \{s \in \mathbb{R} : F(s) < \infty\}$, for any $F \in \mathcal{C}_{-\Delta,\Omega}$. The set $\mathcal{C}_{-\Delta,\Omega}$ is convex and stable under additions and multiplications by a positive constant, *i.e.* $\mathcal{C}_{-\Delta,\Omega}$ is a convex cone.

Example 1. Let $\gamma > \gamma_d \equiv d/2$. Then

$$\sum_{i\in\mathbb{N}} \frac{1}{\lambda_{0,i}^\gamma} < \infty, \tag{4.7}$$

as we shall see below, so that the function

$$F(s) = \begin{cases} s^{-\gamma} & \text{if } s > 0\,, \\ +\infty & \text{if } s \leq 0\,, \end{cases}$$

is in $\mathcal{C}_{-\Delta,\Omega}$ and therefore $(-\Delta)^{-\gamma}$ is a nuclear operator.

Example 2. Let $F : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ be a non-increasing convex function which is non-negative and such that for any $s \geq 0$, large,

$$F(s) \leq \frac{C}{(1+s)^{\varepsilon+d/2}}$$

for some constants C, $\varepsilon > 0$. Hence $F \in \mathcal{C}_{-\Delta,\Omega}$. In fact, we have that

$$\sum_{i\in\mathbb{N}} F(\lambda_{0,i}) \sim \sum_{k\in\mathbb{N}} F(k) \cdot \#A(k),$$

with $A(k) \equiv \{i \in \mathbb{N} : \ k < \lambda_{0,i} < k+1\}$ and, since $\#A(k)$ grows like $k^{d/2-1}$ as $k \to \infty$, it follows that $F(k) \cdot \#A(k)$ behaves like $k^{-1-\varepsilon}$ as $k \to \infty$. Hence $\sum_{i\in\mathbb{N}} F(\lambda_{0,i})$ is finite.

Example 3. In the class of functions of the Example 2 falls

$$F(s) = \int_s^\infty f(t)\, dt$$

where $f : \mathbb{R} \to \mathbb{R}$ is a *Casimir-type function*, *i.e.* a function which is characterized by the following properties:

i) There exists $s_1 \in [-\infty, \infty)$ such that $f(s) = \infty$, $\forall\, s \in (-\infty, s_1)$.

ii) f is continuous on (s_1, ∞).

iii) There exists $s_2 \in (s_1, \infty]$ such that $f(s) > 0, \forall\, s \in (s_1, s_2)$ and $f(s) = 0$, $\forall\, s \geq s_2$.

iv) f is strictly decreasing on (s_1, s_2) .

v) If $s_2 = \infty$, there exists constants $\varepsilon > 0$ and $C > 0$ such that for any $s \geq 0$, large,

$$f(s) \leq \frac{C}{(1+s)^{\varepsilon+2+d/2}} \ . \tag{4.8}$$

Under these conditions $f(-\Delta)$ is also a trace-class operator: see, *e.g.*, [60] if one requires $\varepsilon > 1$. The case $\varepsilon \in (0, 1)$ is more delicate and requires some additional analysis, for instance to define the free energy (see Section 4.2.4).

The function of Example 1 above, the Fermi-Dirac statistics defined for $\alpha > 0$ by

$$f(s) = \int_{\mathbb{R}^d} \frac{dv}{\alpha + e^{s+|v|^2/2}}$$

and the Boltzmann distribution

$$f(s) = e^{-\alpha s}$$

with $\alpha > 0$, are Casimir-type functions. As already mentioned in the introduction, such functions allow to define free energy functionals which are now widely used in various areas of the theory of partial differential equations.

4.2.3. Sobolev-like cones of nuclear operators (*Conos tipo Sobolev de operadores*)

We recall that for any $L \in \mathcal{S}_\infty$, we denote by $\{(\nu_i(L), \psi_i(L))\}_{i\in\mathbb{N}}$ the sequence of eigenelements of L. Here $\{\psi_i(L)\} \subset \mathrm{L}^2(\Omega)$ is a complete orthonormal system of eigenstates.

Definition 4.2. Let $l \in \mathbb{N}$ and $p \in [1, \infty[$. An operator $L \in \mathcal{S}_1$ is in the *Sobolev-like cone* $\mathcal{W}^{l,p}$ if $\{\psi_i(L)\}_{i\in\mathbb{N}} \subset \mathrm{W}_0^{1,p}(\Omega) \cap \mathrm{W}^{l,p}(\Omega)$ and

$$\langle\!\langle L \rangle\!\rangle_{l,p} \equiv \sum_{i\in\mathbb{N}} |\nu_i| \cdot ||\psi_i||^p_{W^{l,p}(\Omega)} < \infty \, . \tag{4.9}$$

The corresponding subset of non-negative operators will be denoted by

$$\mathcal{W}^{l,p}_+ \equiv \{L \in \mathcal{W}^{l,p} : \; L \geq 0\} \, .$$

We also define the functional $\mathcal{K}_p$ on $\mathcal{W}^{1,p}$ by

$$\mathcal{K}_p(L) \equiv \sum_{i\in\mathbb{N}} |\nu_i| \int_\Omega |\nabla\psi_i(x)|^p \, dx \, .$$

Proposition 4.1. *Sobolev-like cones of trace-class operators satisfy the following properties:*

i) *For any $p \in [1, \infty[$, $l \in \mathbb{N}$, $\mathcal{W}^{l,p}$ and $\mathcal{W}^{l,p}_+$ are cones such that*

$$\mathcal{W}^{l_2,p} \subset \mathcal{W}^{l_1,p} \quad \textit{and} \quad \mathcal{W}^{l_2,p}_+ \subset \mathcal{W}^{l_1,p}_+ \quad \textit{if} \quad l_1 \leq l_2 \, .$$

ii) *If* $1 \leq p < q < \infty$, $l \in \mathbb{N}$, *then there exists a constant* $c_1 = c_1(p,q,l)$ *such that*

$$\langle\!\langle L \rangle\!\rangle_{l,p} \leq c_1 \, \langle\!\langle L \rangle\!\rangle_{l,q} \quad \forall\, L \in \mathcal{W}^{l,q}\,,$$

so that $\mathcal{W}^{l,q} \subset \mathcal{W}^{l,p}$.

iii) *For any* $p \geq 2$, *there exists a constant* $c_2 = c_2(\Omega, p)$ *such that*

$$\|L\|_1 \leq c_2 \, \mathcal{K}_p(L), \quad \forall\, L \in \mathcal{W}^{1,p}\,. \tag{4.10}$$

Notice that $c_2(\Omega,p)$ is bounded from above by $c_2(\Omega,2)\,|\Omega|^{1-2/p}$, where $c_2(\Omega,2)$ is Poincaré's constant.

For simplicity, we shall consider only the case $p = 2$ in the rest of this paper and define specifically the corresponding sets as follows.

Definition 4.3. *Trace-class operators with finite kinetic energy.*

$$L \in \mathcal{H}^1 \equiv \mathcal{W}^{1,2} \quad \Longleftrightarrow \quad \begin{cases} L \in \mathcal{S}_1 \\ \psi_i(L) \in \mathrm{H}^1_0(\Omega) \quad \forall i \in \mathbb{N} \\ \sum_{i\in\mathbb{N}} |\nu_i| \cdot \int_\Omega |\nabla \psi_i(L)|^2 dx < \infty \end{cases}$$

$$L \in \mathcal{H}^1_+ \equiv \mathcal{W}^{1,2}_+ \quad \Longleftrightarrow \quad L \in \mathcal{H}^1 \quad \text{and} \quad L \geq 0$$

The *kinetic energy* functional $\mathcal{K} = \mathcal{K}_2$ is linear on the set $\mathcal{H}^1_+$, so that

$$\langle D\mathcal{K}(L), R\rangle = \mathcal{K}(R) \quad \forall\, L, R \in \mathcal{H}^1_+\,,$$

and we shall say that $\mathcal{K}(L)$ is the *kinetic energy* of L. The Sobolev-like cones $\mathcal{H}^1$ and $\mathcal{H}^1_+$ are the analogues of $\mathrm{H}^1(\Omega)$ and $\mathrm{H}^1_+(\Omega) = \{u \in \mathrm{H}^1(\Omega) :\ u \geq 0\}$ at the level of self-adjoint compact operators. This results in integrability properties for the density $\rho_L(x) = \sum_{i\in\mathbb{N}} \nu_i\, |\psi_i(x)|^2$ which are the counterpart of Sobolev's embeddings.

Proposition 4.2. *For any* $L \in \mathcal{H}^1$, *the density function* ρ_L *belongs to* $\mathrm{W}^{1,r}(\Omega) \cap \mathrm{L}^q(\Omega)$ *with* r *and* q *in the following ranges:*

i) *for all* $q \in [1, \infty]$ *and* $r \in [1,2]$ *if* $d = 1$,

ii) *for all* $q \in [1, \infty[$ *and* $r \in [1,2]$ *if* $d = 2$,

iii) *for all* $q \in [1, d/(d-2)]$ *and* $r \in [1, d/(d-1)]$ *if* $d \geq 3$.

Proof. Assume that $d \geq 3$ and $r \in [1, d/(d-1)]$. Using the convexity of $s \mapsto |s|^r$, Hölder's and Sobolev's inequalities, we obtain

$$\begin{aligned}\int_\Omega |\nabla \rho_L|^r \, dx &\leq 2^r \int_\Omega \Big(\sum_{i \in \mathbb{N}} |\nu_i \, \psi_i \, \nabla \psi_i| \Big)^r \, dx \\ &\leq \Big(2 \sum_{j \in \mathbb{N}} |\nu_j| \Big)^r \int_\Omega \sum_{i \in \mathbb{N}} \Big(\tfrac{|\nu_i|}{\sum_{j \in \mathbb{N}} |\nu_j|} \Big) |\psi_i|^r |\nabla \psi_i|^r \, dx \\ &\leq 2^r \Big(\sum_{j \in \mathbb{N}} |\nu_j| \Big)^{r-1} \sum_{i \in \mathbb{N}} |\nu_i| \left(\int_\Omega |\nabla \psi_i|^2 \right)^{\frac{r}{2}} \left(\int_\Omega |\psi_i|^{\frac{2r}{2-r}} \right)^{1-\frac{r}{2}} \\ &\leq 2^r \, s_r^r \, \|L\|_1^{r-1} \, \mathcal{K}(L)\end{aligned}$$

where s_r is the Sobolev constant of the embedding $H_0^1(\Omega) \hookrightarrow L^{\frac{2r}{2-r}}(\Omega)$, so that (4.10) with $c_2 = c_2(\Omega, 2)$ implies

$$||\nabla \rho_L||_{L^r(\Omega)} \leq 2 \, s_r \, \|L\|_1^{1-\frac{1}{r}} \mathcal{K}^{\frac{1}{r}}(L) \leq 2 \, s_r \, c_2^{1-\frac{1}{r}} \, \mathcal{K}(L) \, .$$

Therefore, by the critical Sobolev embedding, we have

$$||\rho_L||_{L^{d/(d-2)}(\Omega)} \leq s_{d/(d-1)} \, ||\nabla \rho_L||_{L^{d/(d-1)}(\Omega)} \leq 2 \, s^2_{d/(d-1)} \, c_2^{1-\frac{1}{r}} \, \mathcal{K}(L) < \infty \, .$$

The cases $d = 1$, 2 follow from the Sobolev inequalities, with the corresponding restrictions on q and r. □

4.2.4. The Free Energy functional (*El funcional de Energía Libre*)

The *free energy functional* is made of an entropy functional and an energy functional, which is itself divided into a kinetic and a potential energy functionals.

Potential energy

Potential energy for trace-class operators can be defined as follows. Let $V : \Omega \to \mathbb{R}$ be a measurable function and let $L \in \mathcal{S}_1$. If $\rho_{|L|} V \in \mathrm{L}^1(\Omega)$, then

$$\mathcal{P}_V(L) \equiv \int_\Omega V(x) \rho_{|L|}(x) \, dx$$

will be called the V-*potential energy of* L.

Since $V = V(x)$ can formally be seen as an operator acting on $L^2(\Omega)$ with kernel $K_V(x,y) = V(x)\,\delta_x(y)$, it follows that $\mathcal{P}(L) = \operatorname{tr}[\,V\,|L|\,]$ and so, at least formally, for any non-negative operators L, $R \in \mathcal{S}_1$,

$$\langle D\mathcal{P}_V(L), R\rangle = \mathcal{P}_V(R)\ .$$

The V-potential energy functional is bounded from below in $\mathcal{H}^1_+$ if and only if V is non-negative. To be precise, we have the following result for any subset of $\mathcal{H}^1_+$ which is stable under multiplication by positive constants.

Proposition 4.3. *Assume that $A \subseteq \mathcal{S}_1$ is such that $\alpha\,A \subseteq A$, for all $\alpha > 0$. Then*

$$\operatorname*{ínf}_{L\in A} \mathcal{P}(L) \geq C$$

for some constant $C \in \mathbb{R}$ if and only if

$$\operatorname*{ínf}_{L\in A} \mathcal{P}(L) = 0\ ,$$

which is equivalent to assume that $V \geq 0$ a.e.

Proof. If $L \in A$ is such that $0 > \mathcal{P}(L) > C$, then it should also be true that

$$0 > \mathcal{P}(\alpha L) = \alpha\,\mathcal{P}(L) > C \quad \forall\,\alpha > 0\ ,$$

which is false if we choose $\alpha > |C|/|\mathcal{P}(L)|$. Reciprocally it is clear that $\operatorname{lím}_{\alpha\to 0}\mathcal{P}(\alpha L) = 0$, and it is easy to find L such that $\mathcal{P}(L) < 0$, $\operatorname{lím}_{\alpha\to\infty}\mathcal{P}(\alpha L) = -\infty$ if V is negative on a measurable set in Ω. □

Entropy

Let $L \in \mathcal{S}_1$ and let $\beta : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ be a convex function such that $\beta(0) = 0$. The functional

$$\mathcal{E}_\beta(L) \equiv \sum_{i\in\mathbb{N}} \beta(\nu_i)$$

will be called the β-*entropy of* L. By convexity, $\mathcal{E}_\beta$ takes values in $(-\infty, +\infty]$. For β of class C^1, since $\mathcal{E}_\beta(L) = \operatorname{tr}[\beta(L)]$, we formally have, for any L, $R \in \mathcal{S}_1$,

$$\langle D\mathcal{E}_\beta(L), R\rangle = \operatorname{tr}[\,\beta'(L)\,R\,]\ .$$

Free energy

The free energy is the sum of the entropy, the kinetic and the potential energies. Here we take temperature 1 from the physics point of view. Assume that $L \in \mathcal{H}^1$ and that $V : \Omega \to \mathbb{R}$ is a measurable function such that $\rho_{|L|} V \in \mathrm{L}^1(\mathbb{R}^d)$.

Definition 4.4.

$$\mathcal{F}_{V,\beta}(L) \equiv \mathcal{E}_\beta(L) + \mathcal{K}(L) + \mathcal{P}_V(L)$$

will be called the (V, β)-*free energy of* L.

Under the above assumptions on V and β, we formally have, for any L, $R \in \mathcal{S}_1$,

$$\langle \mathcal{F}_{V,\beta}(L), R \rangle = \mathrm{Tr}\left[\, \beta'(L)\, R \,\right] + \mathcal{K}(R) + \mathcal{P}_V(R) \ .$$

Example 1. Let $\gamma > \gamma_d \equiv d/2$. We denote by $\mathcal{E}_{\beta_m}$ the entropy corresponding to

$$\beta_m(s) = \begin{cases} \infty & \text{if} \quad s < 0 \ , \\ -\, c_m\, s^m & \text{if} \quad s \geq 0 \ , \end{cases}$$

where $c_m = (1-m)^{m-1} m^{-m}$ and $m = \frac{\gamma}{\gamma+1} \in \left(\frac{d}{d+2}, 1\right)$. Such an entropy will play an important role in Section 4.3.1 below.

Poisson potential energy

Let $d \leq 4$. By virtue of Proposition 4.2, ρ_L is in $\mathrm{L}^2(\Omega)$ for any $L \in \mathcal{H}^1$ so that we can find a potential $V_L \in \mathrm{H}^1_0(\Omega)$, called the *Poisson potential*, as the unique solution of the equation

$$\begin{cases} -\Delta V = \varepsilon\, \rho_{|L|}, & \text{in} \quad \Omega; \\ \quad V = 0, & \text{on} \quad \partial\Omega \end{cases}$$

Two cases can be considered, corresponding either to the repulsive, electrostatic case: $\varepsilon = +1$ (Coulomb interaction), or to the attractive case: $\varepsilon = -1$ (Newton interaction). The *Poisson potential energy* of $L \in \mathcal{H}^1$,

$$\mathcal{P}(L) = \frac{1}{2} \int_\Omega V_L\, \rho_L\, dx = \frac{\varepsilon}{2} \int_\Omega |\nabla V_L|^2\, dx \ ,$$

is then well defined. Using Proposition 4.2 we get the following regularity properties.

Proposition 4.4. *Let $L \in \mathcal{H}^1$. If $d = 1$ or $d = 2$, then $V_L \in \mathrm{C}^0(\overline{\Omega})$. Moreover, $V_L \in \mathrm{W}_0^{1,p}(\Omega) \cap \mathrm{L}^q(\Omega)$ for any $q \in [1, \infty)$ and for any $p \in [1, \infty)$ if $d = 3$, for any $p \in [1, 4]$ if $d = 4$. If additionally $\partial\Omega$ is of class C^2, then $V_L \in \mathrm{W}^{2,r}(\Omega) \cap \mathrm{C}^{0,1/2}(\Omega)$ for any $r \in [1, 3/2]$ if $d = 3$, and $V_L \in \mathrm{W}^{2,r}(\Omega)$ for any $r \in [1, 4/3]$ if $d = 4$.*

Such a result is classical. We refer the interested reader for instance to [41] for more details. The most general free energy functional now is $\mathcal{F}_{V,\beta}(L) + \mathcal{P}(L)$. Such a functional is convex if $\varepsilon = +1$, but not any more if $\varepsilon = -1$.

4.3. Main results (*Resultados principales*)

4.3.1. Lieb-Thirring and Gagliardo-Nirenberg inequalities (I) (*Desigualdades de Lieb-Thirring y Gagliardo-Nirenberg (I)*)

Here we translate the results of [26] into the operators formalism and adapt results originally written in $\mathbb{R}^d$ to a domain $\Omega \subset \mathbb{R}^d$. We shall denote by $\{\lambda_{V,i}\}_{i\in\mathbb{N}}$ and $\{\phi_{V,i}\}_{i\in\mathbb{N}}$ respectively the sequence of eigenvalues of $-\Delta+V$ and a corresponding $\mathrm{L}^2(\Omega)$-orthonormal sequence of eigenstates, where $V = V(x)$ is some given potential.

Let f be a nonnegative function on $\mathbb{R}^+$ such that

$$\int_0^\infty f(t)\,\left(1 + t^{-d/2}\right)\,\frac{dt}{t} < \infty \tag{4.11}$$

and define

$$F(s) := \int_0^\infty e^{-t\,s}\, f(t)\,\frac{dt}{t} \quad \text{and} \quad G(s) := \int_0^\infty e^{-t\,s}\,(4\pi\,t)^{-d/2}\, f(t)\,\frac{dt}{t}\,. \tag{4.12}$$

Notice that if d is even,

$$(-4\pi)^{\frac{d}{2}}\,\frac{d^{\frac{d}{2}}G}{ds^{\frac{d}{2}}}(s) = F(s)\,.$$

The following result has been proved in [26, Section 2]. If $V \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ is non-negative and $G(V) \in L^1(\mathbb{R}^d)$, and if f satisfies Assumption (4.11), then

$$\mathrm{Tr}\left[F\left(-\Delta + V\right)\right] \le \int_{\mathbb{R}^d} G(V(x))\,dx\,.$$

In the case of a domain $\Omega \subset \mathbb{R}^d$, formally extending V to $\mathbb{R}^d \setminus \Omega$ by ∞, we can deduce the following result. A rigorous proof is easily achieved by taking an appropriate approximation procedure.

Corollary 4.1. *Let V be a non-negative potential in $L^1_{\rm loc}(\Omega)$. Assume moreover that $G(V)$ is in $L^1(\Omega)$. With F and G defined by (4.11)-(4.12), if f satisfies Assumption (4.11), there exists a constant $C < 1$ such that*

$$\sum_{i\in\mathbb{N}} F(\lambda_{V,i}) = \mathrm{Tr}\left[F\left(-\Delta + V\right)\right] \leq C \int_\Omega G(V(x))\,dx\ .$$

Notice that $C = C(\Omega)$ depends on Ω and that $\text{ínf}_\Omega C(\Omega) = 1$, where the infimum is taken on all domains $\Omega \subset \mathbb{R}^d$ with smooth boundary. The only point to be proved is that $C < 1$. This is left to the reader. Also notice that since V is assumed to be non-negative, the sequence $\{\lambda_{V,i}\}_{i\in\mathbb{N}}$ has only positive elements and diverges since $\lambda_{V,i} \geq \lambda_{0,i}$ for any $i \in \mathbb{N}$. If F is C^1, convex, on $\mathbb{R}^+$, then F is in the $\mathcal{C}_{-\Delta,\Omega}$ class (see Definition 4.1) since $\text{lím}_{s\to\infty} F(s) = 0$ can be achieved only if F is non-increasing. The fact that V is non-negative looks rather restrictive but can be overcome in cases of practical interest for instance as follows.

Corollary 4.2. *Let V be in $L^1_{\rm loc}(\Omega)$. Assume that F and G are defined by (4.11)-(4.12), and that f satisfies Assumption (4.11). If V is bounded from below, then, for any $\lambda < \mathrm{infess}_\Omega V$ such that $G(V-\lambda)$ is in $L^1(\Omega)$,*

$$\sum_{i\in\mathbb{N}} F(\lambda_{V,i} - \lambda) = \mathrm{Tr}\left[F\left(-\Delta + V - \lambda\right)\right] \leq C \int_\Omega G(V(x) - \lambda)\,dx\ .$$

The constant C is the same as in Corollary 4.1. These two corollaries can be illustrated by the following examples.

Example 1. If, for any $s \geq 0$, $F(s) \equiv s^{-\gamma}$, then $G(s) \equiv (4\pi)^{-d/2}\,\Gamma(\gamma - \frac{d}{2})\, s^{\frac{d}{2}-\gamma}/\Gamma(\gamma)$. In such a case, Corollary 4.1 takes the special following form:

$$\mathrm{Tr}\left[(-\Delta + V)^{-\gamma}\right] = \sum_{i\in\mathbb{N}} (\lambda_{V,i})^{-\gamma} \leq \frac{\Gamma(\gamma - \frac{d}{2})}{(4\pi)^{d/2}\,\Gamma(\gamma)} \int_\Omega V^{\frac{d}{2}-\gamma}\,dx\ .$$

Example 2. If, for any $s \in \mathbb{R}$, $F(s) \equiv e^{-s}$, then $G(s) \equiv (4\pi)^{-d/2}\,e^{-s}$. Corollary 4.2 applies as follows. Notice that e^λ appears on both sides of the inequality, so it simplifies and then, using a density argument, the condition that V is bounded from below can be removed.

Corollary 4.3. *There exists a constant $C < 1$ such that for any $V \in L^1_{\mathrm{loc}}(\Omega)$ such that $e^{-V} \in L^1(\Omega)$, we have*

$$\mathrm{Tr}\left[e^{-\Delta+V}\right] = \sum_{i\in\mathbb{N}} e^{-\lambda_{V,i}} \leq \frac{C}{(4\pi)^{d/2}} \int_\Omega e^{-V}\, dx\ .$$

We will see later how to directly prove results in the general case when V does not have a definite sign.

Given a function $\theta : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ such that $\theta \not\equiv +\infty$, we shall denote by θ^* the Legendre-Fenchel transform of θ, *i.e.*, the function defined by

$$\theta^*(\nu) \equiv \sup_{\lambda\in\mathbb{R}} \{\nu\lambda - \theta(\lambda)\}, \quad \forall\, \nu \in \mathbb{R}\ .$$

From $\beta(s) \equiv F^*(-s)$, we get

$$\beta(\nu) + \nu\,\lambda \geq -F(\lambda), \quad \forall\, \nu,\, \lambda \in \mathbb{R}\ , \tag{4.13}$$

with equality if (resp. if and only if) F is convex (resp. strictly convex). In terms of operators, this means

$$\mathcal{F}_{V,\beta}(L) \geq -\mathrm{Tr}\left[F(-\Delta + V)\right], \quad \forall\, L \in \mathcal{H}^1_+\ . \tag{F}$$

Hence we get a uniform lower bound for $\mathcal{F}_{V,\beta}$ on $\mathcal{H}^1_+$ under the conditions of Corollary 4.1. If for some convex function $G \in \mathrm{C}^0(\Omega)$, for instance given in terms of F as in Corollary 4.1, we have

$$-\mathrm{Tr}\left[F(-\Delta + V)\right] \geq -\int_\Omega G(V(x))\, dx\ , \tag{G}$$

then, for all $L \in \mathcal{H}^1_+$,

$$\mathcal{E}_\beta(L) + \mathcal{K}(L) + \mathcal{J}_L(V) = \mathcal{F}_{V,\beta}(L) + \int_\Omega G(V(x))\, dx \geq 0$$

where

$$\mathcal{J}_L(V) \equiv \int_\Omega \left[V(x)\rho_L(x) + G(V(x))\right] dx\ .$$

Now, as in [26], for L fixed we optimize $\mathcal{J}_L(\cdot)$ in the set of potentials V which verify (F) and (G). If V_0 is a critical point of $\mathcal{J}_L(\cdot)$, then

$$G'(V_0) + \rho_L = 0\ .$$

By defining $\tau(s) \equiv -\big[\big(G \circ (G')^{-1}\big)(-s) + s\,(G')^{-1}(-s)\big]$, *i.e.* for τ such that

$$G(s) = \tau^*(-s)\,,$$

we have that

$$\mathcal{J}_L(V_0) = -\int_\Omega \tau(\rho_L(x))\,dx$$

and can state the following

Theorem 4.3. *Let F and G be defined by Assumptions (4.11)-(4.12), and consider β and τ such that $\beta(s) \equiv F^*(-s)$ and $G(s) \equiv \tau^*(-s)$. Under Assumptions (F) and (G), for any $L \in \mathcal{H}^1_+$, we have*

$$\mathcal{K}(L) + \mathcal{E}_\beta(L) \geq C\int_\Omega \tau\left(\frac{\rho_L}{C}\right)\,dx\,.$$

This provides interesting insights in the following two typical examples.

Example 1. Assume that $\gamma > \gamma_d \equiv d/2$ and consider the convex function $\beta_m(s) = -\,c_m\,s^m$ on $\mathbb{R}^+$, extended by $+\infty$ on $(-\infty,0)$, where $c_m = (1-m)^{m-1}m^{-m}$, $m = \frac{\gamma}{\gamma+1} \in]\frac{d}{d+2},1[$. The corresponding functions $F(s) \equiv \beta_m^*(-s)$ extended by $+\infty$ on $(-\infty,0)$ and G take the form: $F(s) \equiv s^{-\gamma}$ and $G(s) \equiv (4\pi)^{-d/2}\,\Gamma(\gamma-\frac{d}{2})\,s^{\frac{d}{2}-\gamma}/\Gamma(\gamma)$ for any $s \geq 0$. Define $q \equiv (2\gamma-d)/(2(\gamma+1)-d) \in (0,1)$. In such a case, Theorem 4.3 takes the special following form.

Corollary 4.4. *With the above notations, for any $L \in \mathcal{H}^1_+$,*

$$\mathcal{K}(L) + \kappa(\gamma)\int_\Omega \rho_L^q\,dx \geq c_m\,\mathrm{Tr}\,[L^m]\ ,$$

where $\kappa(\gamma) \equiv (C\,\mathcal{C}(\gamma))^{1-q}\,[(\frac{q}{q-1})^{1-q} + (\frac{q}{q-1})^{-q}]$.

Example 2. Consider the convex function $\beta_1(s) \equiv s\log s - s$ if $s > 0$, extended by $\beta_1(0) = 0$ and $+\infty$ on $(-\infty,0)$, and $F(s) \equiv e^{-s}$, $G(s) \equiv (4\pi)^{-d/2}\,e^{-s}$ for any $s \in \mathbb{R}$. Theorem 4.3 applies as follows.

Corollary 4.5. *For any $L \in \mathcal{H}^1_+$,*

$$\mathcal{K}(L) + \mathrm{Tr}\,[L\,\log L] \geq \int_\Omega \rho_L \log\rho_L\,dx + \left[\frac{d}{2}\,\log(4\pi) - \log C\right]\int_\Omega \rho_L\,dx\,.$$

4.3.2. Convexity Estimates (*Estimaciones convexas*)

In [60, Lemma 3] for some special functions F generated by a Casimir-type functions f, in presence of a repulsive Poisson coupling and for $d = 3$ (see Example 3 in Section 4.2.2 above), it has been proved that $\mathcal{F}_{V,\beta} \geq -\mathrm{Tr}\,[F(-\Delta)]$. We first establish a more general result in presence of a non-negative potential V. Here ε is a positive parameter, that will later take values in $(0, 1)$ in case of a sign-changing potential. By $F \in \mathcal{C}_{-\varepsilon\Delta,\Omega}$, we mean that F is convex and, with the notations of (4.6), $\sum_{i\in\mathbb{N}} F(\varepsilon\,\lambda_{0,i})$ is finite. Notice that this implies that $\lim_{\lambda\to\infty} F(\lambda) = 0$, and hence F has to be non-increasing and non-negative.

<u>Lemma</u> 4.1. *Assume that V is a non-negative potential. For any $\psi \in \mathrm{H}^1_0(\Omega)$ such that $||\psi||_{L^2(\Omega)} = 1$, we have*

$$F\Big(\varepsilon\int_\Omega |\nabla\psi|^2\,dx + \int_\Omega V\,|\psi|^2\,dx\Big) \leq (\psi,\, F(-\varepsilon\Delta + V)\,\psi)_{\mathrm{L}^2(\Omega)} \quad \forall\,\varepsilon > 0\;,$$

with equality if ψ is an eigenstate of $-\Delta$. As a consequence, if $F \in \mathcal{C}_{-\varepsilon\Delta,\Omega}$, with $\beta(s) \equiv F^*(-s)$, for any $L \in \mathcal{H}^1_+$ and any $\varepsilon > 0$, we have

$$\mathcal{E}_\beta(L) + \varepsilon\,\mathcal{K}(L) + \mathcal{P}_V(L) \geq -\mathrm{Tr}\,[F(-\varepsilon\Delta + V)]\;.$$

As a consequence, if $F \in \mathcal{C}_{-(1-\varepsilon)\Delta,\Omega}$, for any $L \in \mathcal{H}^1_+$ and any $\varepsilon \in (0, 1]$,

$$\mathcal{F}_{V,\beta}(L) \geq \varepsilon\,\mathcal{K}(L) - \mathrm{Tr}\,[F(-(1-\varepsilon)\,\Delta + V)]\;.$$

Proof. Let $\varepsilon > 0$ and consider $\{(\lambda_{0,i}, \phi_{0,i})\}_{i\in\mathbb{N}}$ as in (4.6). There exists a sequence $\{\alpha_i\}_{i\in\mathbb{N}} \subset \mathbb{R}$ such that $\psi = \sum_{i\in\mathbb{N}} \alpha_i\,\phi_{0,i}$ and $\sum_{i\in\mathbb{N}} \alpha_i^2 = 1$. By convexity of F, we obtain

$$\begin{aligned} F\Big(\varepsilon\int_\Omega |\nabla\psi|^2\,dx + \int_\Omega V\,|\psi|^2\,dx\Big) &= F\Big(\varepsilon\sum_{i\in\mathbb{N}} \alpha_i^2\,\lambda_{0,i}\Big) \\ &\leq \sum_{i\in\mathbb{N}} \alpha_i^2\,F(\varepsilon\,\lambda_{0,i}) = (\psi,\, F(-\varepsilon\Delta + V)\,\psi)_{\mathrm{L}^2(\Omega)}\;. \end{aligned}$$

If ψ is an eigenstate of $-\Delta$, with no restriction we may assume that $\psi = \phi_{0,i_0}$ for some $i_0 \in \mathbb{N}$, so that $\alpha_i = \delta_{i,i_0}$ for any $i \in \mathbb{N}$. The above inequality becomes an equality.

Using (4.13), we can bound from below the free energy: Substituting ν_i for ν, $\varepsilon \int_\Omega |\nabla\psi_i|^2\, dx$ for λ and summing over $i \in \mathbb{N}$, we get

$$\begin{aligned}\mathcal{E}_\beta(L) + \varepsilon\, \mathcal{K}(L) + \mathcal{P}(L) &= \sum_{i\in\mathbb{N}} \Big[\beta(\nu_i) + \nu_i \int_\Omega \big(\, \varepsilon\, |\nabla\psi_i|^2 + V\, |\psi_i|^2 \,\big)\, dx\Big] \\ &\geq -\sum_{i\in\mathbb{N}} F\Big(\varepsilon \int_\Omega |\nabla\psi_i|^2\, dx + \int_\Omega V\, |\psi_i|^2\, dx\Big) \\ &\geq -\sum_{i\in\mathbb{N}} (\psi_i,\, F(-\varepsilon\Delta + V)\, \psi_i)_{\mathrm{L}^2(\Omega)} = -\mathrm{Tr}\,[F(-\varepsilon\Delta)]\ .\end{aligned}$$

□

We can extend our approach to potentials which take negative values as follows. For this purpose, some additional definitions are needed.

Definition 4.5. We will say that the Schrödinger operator $-\Delta + V$ is *ε coercive* for some $\varepsilon \in (0, 1]$ if and only if

$$\lambda^\varepsilon_{V,1} \equiv \sup\{\mu \in \mathbb{R}\ :\ -(1-\varepsilon)\,\Delta + V \geq \mu\} > -\infty \qquad (\mathrm{C}_\varepsilon)$$

The ε coercivity indeed means that

$$-\Delta + V - \lambda^\varepsilon_{V,1} \geq -\varepsilon\,\Delta$$

in the sense of operators. We will denote by $\{\lambda^\varepsilon_{V,i}\}_{i\in\mathbb{N}}$ the sequence of eigenvalues of the operator $-(1-\varepsilon)\,\Delta + V$, if this operator has only pure point spectrum. Notice that $\lambda^0_{V,1} = \lambda_{V,1}$ while Condition (C_ε) for $\varepsilon = 1$ means that V is nonnegative a.e. by Proposition 4.3. For each $\lambda \leq \lambda^\varepsilon_{V,1}$ and each convex function F, we define $\mathcal{F}^\lambda_{V,\beta} : \mathcal{H}^1 \to \mathbb{R} \cup \{\infty\}$ by

$$\mathcal{F}^\lambda_{V,\beta}(L) \equiv \mathcal{F}_{V,\beta}(L) - \lambda\, \|L\|_1\ .$$

Definition 4.6. We shall say that a function $F : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ is of $\mathcal{C}^{\lambda,\varepsilon}_{-(1-\varepsilon)\Delta+V,\Omega}$*-class* if it is convex and $\sum_{i\in\mathbb{N}} F(\lambda^\varepsilon_{V,i} - \lambda)$ is finite.

If $F \in \mathcal{C}^{\lambda,\varepsilon}_{-(1-\varepsilon)\Delta+V,\Omega}$, then $[\lambda^\varepsilon_{V,1} - \lambda, \infty) \subset \mathrm{Dom}(F)$ even if $V - \lambda$ has a non-trivial negative component. With the same convexity argument as in the proof of Lemma 4.1, we can see that if V verifies Condition (C_ε) for a given $\varepsilon \in [0, 1]$, then for any $F \in \mathcal{C}^{\lambda,\varepsilon}_{-(1-\varepsilon)\Delta+V,\Omega}$ and any $\lambda \leq \lambda^\varepsilon_{V,1}$,

$$\mathcal{F}^\lambda_{V,\beta}(L) \geq \varepsilon\, \mathcal{K}(L) - \mathrm{Tr}\,[F(-(1-\varepsilon)\,\Delta + V - \lambda)] \quad \forall\, L \in \mathcal{H}^1\ ,$$

so that $\mathcal{F}^\lambda_{V,\beta}(L)$ is uniformly bounded from below and coercive by (4.10), in the sense that $\|L\|_1$ is uniformly bounded in terms of $\mathcal{F}^\lambda_{V,\beta}(L)$.

It is easy to check that if V is non-negative, then $\mathcal{C}^{\lambda,\varepsilon}_{-(1-\varepsilon)\Delta+V,\Omega} \subset \mathcal{C}_{-(1-\varepsilon)\Delta,\Omega}$ for any $\lambda < 0$. It turns out that $\mathcal{F}^\lambda_{V,\beta}(L)$ is still bounded from below and coercive under Condition (C_ε) even if $(V-\lambda)_-$ is non-trivial, as shown by the following result.

Proposition 4.5. *Let V be a potential verifying (C_ε) for some $\varepsilon \in (0,1]$. For any $F \in \mathcal{C}_{-\frac{\varepsilon}{2}\Delta,\Omega}$, let $\beta(s) \equiv F^*(-s)$, $s \in \mathbb{R}$. For any $\lambda \leq \lambda^\varepsilon_{V,1}$, for any $L \in \mathcal{H}^1$,*

$$\mathcal{F}^\lambda_{V,\beta}(L) \geq -\mathrm{Tr}\left[F\left(-\frac{\varepsilon}{2}\Delta\right)\right] + \frac{\varepsilon}{2}\mathcal{K}(L)\ .$$

Hence $\mathcal{F}^\lambda_{V,\beta}$ is bounded from below and coercive, $\mathcal{E}_\beta$ is bounded in terms of $\mathcal{F}^\lambda_{V,\beta}$ and

$$\mathcal{F}^\lambda_{V,\beta}(L) \geq \mathrm{Tr}\left[F(-\Delta+V-\lambda)\right] \quad \forall\, L \in \mathcal{H}^1\ .$$

Moreover, if $\mathcal{F}^\lambda_{V,\beta}(L)$ is finite for some $L \in \mathcal{H}_1$, then $\mathcal{C}_{-\Delta+V,\Omega} \subset \mathcal{C}_{-\varepsilon\Delta,\Omega}$, and $-\Delta+V$ has only pure point spectrum provided F is positive on $(0,+\infty)$.

Proof. Let $L \in \mathcal{H}^1$ and decompose $\mathcal{F}^\lambda_{V,\beta}(L)$ as

$$\left(\mathcal{E}_\beta(L) + \frac{\varepsilon}{2}\mathcal{K}(L)\right) + \frac{\varepsilon}{2}\mathcal{K}(L) + \left((1-\varepsilon)\,\mathcal{K}(L) + \mathcal{P}_V(L) - \lambda\,\|L\|_1\right).$$

From Lemma 4.1 we have that

$$\mathcal{E}_\beta(L) + \frac{\varepsilon}{2}\mathcal{K}(L) \geq -\mathrm{Tr}\left[F\left(-\frac{\varepsilon}{2}\Delta\right)\right]\ .$$

On the other hand, from (C_ε) it follows that

$$\begin{aligned}&(1-\varepsilon)\,\mathcal{K}(L) + \mathcal{P}_V(L) - \lambda\,\|L\|_1\\ &\qquad = \sum_{i\in\mathbb{N}} |\nu_i| \int_\Omega \left((1-\varepsilon)\,|\nabla\psi_i|^2 + (V-\lambda)\,|\psi_i|^2\right) dx \geq 0\ ,\end{aligned}$$

where $\psi_i = \psi_i(L)$ with the notations of Section 4.2.1. The bound on $\mathcal{E}_\beta$ follows from the decomposition of $\mathcal{F}^\lambda_{V,\beta}(L)$ and Lemma 4.1. This proves the lower bound on $\mathcal{F}^\lambda_{V,\beta}(L)$ and the upper bound on $\mathcal{E}(L)$.

A minimum of $\mathcal{F}^\lambda_{V,\beta}(L)$ on $\mathcal{H}_1$, which is achieved as we shall see later, is given by

$$\beta'(\nu_i) = \lambda - \lambda^0_{V,i}\ ,$$

so that

$$\inf_{L\in\mathcal{H}^1}\left(\mathcal{F}^{\lambda}_{V,\beta}(L)\right)=\mathrm{Tr}\left[F(-\Delta+V-\lambda)\right]$$

is finite. The assertion on the spectrum of $-\Delta+V$ easily follows. Notice that from its definition, F is non-negative. Since $\sum_{i\in\mathbb{N}}F(\lambda^{\varepsilon}_{V,i})<\infty$, to prove that $\{\lambda^{\varepsilon}_{V,i}\}_{i\in\mathbb{N}}$ diverges, it is therefore sufficient to require that F is positive. □

Corollary 4.6. *Under the conditions of Proposition 4.5, if $\{L_\sigma\}_{\sigma\in\Sigma}$ is a family in $\mathcal{H}^1_+$ such that $\{\mathcal{F}^{\lambda}_{V,\beta}(L_\sigma)\}_{\sigma\in\Sigma}$ is bounded, then the families $\{\|L_\sigma\|_1\}_{\sigma\in\Sigma}$, $\{K(L_\sigma)\}_{\sigma\in\Sigma}$, $\{\mathcal{E}_\beta(L_\sigma)\}_{\sigma\in\Sigma}$ and $\{\mathcal{P}_V(L_\sigma)\}_{\sigma\in\Sigma}$ are also bounded.*

Proof. As follows from the proof of Proposition 4.5, it is clear that the boundedness of $\mathcal{F}^{\lambda}_{V,\beta}(L_\sigma)$ implies the boundedness from above of $(1-\varepsilon)\,\mathcal{K}(L_\sigma)+\mathcal{P}_V(L_\sigma)-\lambda\,\|L_\sigma\|_1$ which, in its turn, together with the boundedness from above of $\mathcal{E}_\beta$, implies the boundedness from above of $\mathcal{K}(L_\sigma)$ and therefore (see (4.10)) that of $\|L_\sigma\|_1$. The boundedness of $\mathcal{E}_\beta(L_\sigma)$ and of $\mathcal{P}_V(L_\sigma)$ follows. □

4.3.3. Lieb-Thirring and Gagliardo-Nirenberg inequalities (II) (*Desigualdades de Lieb-Thirring y Gagliardo-Niremberg (II)*)

In Section 4.3.1, Gagliardo-Nirenberg inequalities have been established only for nonnegative potentials. Under Condition (C_ε) for some $\varepsilon\in(0,1)$, an interpolation inequality also holds in presence of a sign changing potential. To start with, we use a scaling to rewrite Corollary 4.1 with $-\Delta$ replaced by $-\varepsilon\Delta$.

Lemma 4.2. *Let $\varepsilon\in(0,1)$ and consider a non-negative potential W. Let F and G be defined by Assumptions (4.11)-(4.12), and consider β and τ such that $\beta(s)\equiv F^*(-s)$ and $G(s)\equiv\tau^*(-s)$, with the notations of Section 4.3.1. Then, for any $L\in\mathcal{H}^1_+$,*

$$\mathrm{Tr}\left[\beta(L)+(-\varepsilon\Delta+W)L\right]\geq-\mathrm{Tr}\left[F(-\varepsilon\Delta+W)\right]\geq-\,\varepsilon^{-\frac{d}{2}}\int_\Omega G(W)\;dx\;.$$

Proof. Let $\psi_i=\psi_i(L)$, $i\in\mathbb{N}$, and consider $\psi_i^\varepsilon(x)=\varepsilon^{d/4}\psi_i(\sqrt{\varepsilon}\,x)$, $W^\varepsilon(x)=W(\sqrt{\varepsilon}\,x)$ for any $x\in\varepsilon^{-1/2}\,\Omega$. Hence

$$\int_\Omega\left(\varepsilon\,|\nabla\psi_i|^2+W\,|\psi_i|^2\right)\,dx=\int_{\varepsilon^{-1/2}\,\Omega}\left(\,|\nabla\psi_i^\varepsilon|^2+W^\varepsilon\,|\psi_i^\varepsilon|^2\right)\,dx\;,$$

$$\mathrm{Tr}\left[\beta(L) + (-\varepsilon\Delta + W)L\right] \geq \mathrm{Tr}\left[\beta(L^\varepsilon) + (-\varepsilon\Delta + W^\varepsilon)L^\varepsilon\right]$$

with evident notations, and the results of Corollary 4.1 apply:

$$\mathrm{Tr}\left[\beta(L^\varepsilon) + (-\varepsilon\Delta + W^\varepsilon)L^\varepsilon\right] \geq -\mathrm{Tr}\left[F(-\Delta + W^\varepsilon)\right] \geq -\int_{\varepsilon^{-1/2}\,\Omega} G(W^\varepsilon)\, dx\,.$$

The conclusion then holds by undoing the change of variables. Notice here that we apply Corollary 4.1 with $C = 1$ in order to get a constant which does not depend on Ω. □

From Proposition 4.5, we know that $\mathcal{F}^{\lambda}_{V+W,\beta}(L) \geq \mathcal{F}^{\lambda}_{V,\beta}(L)$ is bounded from below for any non-negative W. Hence we can simply write that

$$\mathcal{F}^{\lambda^\varepsilon_{V,1}}_{V+W,\beta}(L) = \mathrm{Tr}\left[(-(1-\varepsilon)\Delta + V - \lambda^\varepsilon_{V,1})L\right] + \mathrm{Tr}\left[\beta(L) + (-\varepsilon\Delta + W)L\right]$$

is bounded from below by $-\,\varepsilon^{-\frac{d}{2}}\int_\Omega G(W)\, dx$, and then we can rearrange this estimate as

$$\mathrm{Tr}\left[\beta(L) + (-\Delta + V - \lambda^\varepsilon_{V,1})L\right] \geq -\int_\Omega \left(\rho_L\, W + \varepsilon^{-\frac{d}{2}}\, G(W)\right)\, dx\,.$$

Optimizing on W as in section Section 4.3.1, we get that the right hand side is bounded from below by

$$\varepsilon^{-\frac{d}{2}} \int_\Omega \tau\left(\varepsilon^{\frac{d}{2}}\,\rho_L(x)\right)\, dx\,,$$

which completes the proof of Theorem 4.1.

4.3.4. Compactness results (*Resultados de compacidad*)

To avoid technicalities, we will assume that the potential is nonnegative. The general case can be dealt with almost with the same arguments, simply by replacing $-\Delta$ by $-\varepsilon\Delta$ and using the fact that $-(1-\varepsilon)\Delta + V - \lambda$ is a nonnegative operator. Details are left to the reader.

Let us start with some observations. Assume that $\{L_n\}_{n\in\mathbb{N}^*}$ is a bounded sequence in $\mathcal{S}_1$ and denote respectively by $\{\nu_i^n\}_{i\in\mathbb{N}}$ and $\{\psi_i^n\}_{i\in\mathbb{N}}$ the sequence of eigenvalues and a sequence of orthonormalized eigenfunctions of L_n. For any $i \in \mathbb{N}$, $n \in \mathbb{N}^*$,

$$\begin{cases} L_n\psi_i^n = \nu_i^n\psi_i^n \\ \left(\psi_i^n,\, \psi_j^n\right)_{\mathrm{L}^2(\Omega)} = \delta_{i,j}, \quad \forall\, j \in \mathbb{N} \end{cases}$$

where $\delta_{i,j}$ is Kronecker's delta symbol. Then there exists a constant $C > 0$ such that $|\nu_i^n| \leq C$, for all $i \in \mathbb{N}$, $n \in \mathbb{N}^*$ and, consequently, there exists a sequence of real numbers $\{\bar{\nu}_i\}_{i\in\mathbb{N}}$ such that, up to the extraction of a subsequence,

$$\lim_{n\to\infty} \nu_i^n = \bar{\nu}_i, \quad \forall\, i \in \mathbb{N}\ .$$

Our first result is concerned with the case of Example 1 in Section 4.3.1.

<u>Theorem</u> 4.4. *Consider a domain Ω in $\mathbb{R}^d$, $d \geq 2$, and assume that $m \in (\frac{d}{d+2}, 1)$. Let $\{L_n\}_{n\in\mathbb{N}^*}$ be a sequence in $\mathcal{H}^1$ such that*

$$K_\infty \equiv \sup_{n\in\mathbb{N}^*} \mathcal{K}(L_n) < \infty\ .$$

for some constant $K_\infty > 0$. Then, $\{L_n\}_{n\in\mathbb{N}^*}$ is bounded in $\mathcal{S}_1$ and, if $\{\nu_i^n\}_{i\in\mathbb{N}}$ is the spectrum of L_n, then

$$\sup_{n\in\mathbb{N}^*} \sum_{i\in\mathbb{N}} |\nu_i^n|^m < \infty\ .$$

Moreover, the following properties hold:

i) *If $\bar{\nu}_i \neq 0$ for all $i \in \mathbb{N}$, then, up to the extraction of a subsequence,*

$$\lim_{n\to\infty} \sum_{i\in\mathbb{N}} |\nu_i^n|^m = \sum_{i\in\mathbb{N}} |\bar{\nu}_i|^m\ .$$

ii) *For any $m' \in (m, 1)$, up to the extraction of a subsequence,*

$$\lim_{n\to\infty} \sum_{i\in\mathbb{N}} |\nu_i^n|^{m'} = \sum_{i\in\mathbb{N}} |\bar{\nu}_i|^{m'}\ .$$

iii) *Up to the extraction of a subsequence, $\{L_n\}_{n\in\mathbb{N}^*}$ converges in $\mathcal{S}_1$.*

Proof. By (4.10), $\sup_{n\in\mathbb{N}^*} \|L_n\|_1 < \infty$. For $i \in \mathbb{N}$, $n \in \mathbb{N}$, let

$$E_i^n \equiv \int_\Omega |\nabla \psi_i^n(x)|^2\, dx\ .$$

The uniform bound on $\|L_n\|_1$ and $\sum_{i\in\mathbb{N}} |\nu_i^n|^m$ follow from Proposition 4.2 and Corollary 4.4 respectively.

Proof of i) Assume first that $\bar{\nu}_i \neq 0$ for any $i \in \mathbb{N}$. Then, for each $i \in \mathbb{N}$, the sequence $\{E_i^n\}_{n\in\mathbb{N}}$ is bounded and, consequently, there is a function $\bar{\psi}_i \in \mathrm{L}^2(\Omega)$ for which, up to a subsequence,

$$\lim_{n\to\infty} \psi_i^n = \bar{\psi}_i \quad \text{in } \mathrm{L}^2(\Omega) .$$

After a reordering we have, counting multiplicity, that $|\bar{\nu}_1| \geq |\bar{\nu}_2| \geq ...$ We denote by $P_N : L^2(\Omega) \to F_N$ the orthogonal projection operator over

$$F_N \equiv \mathrm{span}\{\bar{\psi}_i \ : \ 1 \leq i \leq N-1\}$$

and let $Q_N \equiv I_d - P_N$ be the projection operator onto $F_N^{\perp}$.

Next we claim that for all $\varepsilon > 0$, there exists $N \in \mathbb{N}$ such that

$$\sum_{i=N}^{\infty} |\nu_i^n|^m \leq \varepsilon \quad \forall\, n \in \mathbb{N}^* . \tag{4.14}$$

This can be proved as follows. First, using (4.7), we choose $N \in \mathbb{N}$ such that

$$\left(\sum_{\ell=N}^{\infty} (\lambda_{0,\ell})^{-\gamma}\right)^{m/\gamma} \quad \leq \quad \frac{\varepsilon}{2}$$

where $\gamma = \frac{m}{1-m}$ and $\{\lambda_{0,i}\}_{i\in\mathbb{N}}$ is the sequence of the eigenvalues of $-\Delta$ in $\mathrm{H}_0^1(\Omega)$, with associated eigenfunctions $\phi_{0,i}$, $i \in \mathbb{N}$. Consider for each $n \in \mathbb{N}$ the expansion

$$\psi_i^n = \sum_{k=1}^{\infty} \alpha_{i,k}^n\, \phi_{0,k} \quad n \in \mathbb{N} , \tag{4.15}$$

where $\alpha_{i,k}^n \equiv (\psi_i^n,\, \phi_{0,k})_{\mathrm{L}^2(\Omega)}$. According to the reverse Hölder inequality, *i.e.*, for any $p \in (0,1)$, $q \in (-\infty, 0)$ such that $\frac{1}{p} + \frac{1}{q} = 1$,

$$\sum_{i\in\mathbb{N}} a_i\, b_i \geq \left(\sum_{i\in\mathbb{N}} a_i^p\right)^{1/p} \left(\sum_{i\in\mathbb{N}} b_i^q\right)^{1/q} , \quad \forall\, \{a_i\}_{i\in\mathbb{N}},\, \{b_i\}_{i\in\mathbb{N}} \in (\mathbb{R}^+)^{\mathbb{N}},$$

applied for $p = m = \gamma/(\gamma+1)$, $q = -\gamma$, $a_i = |\nu_i^n|$ and $b_i = E_i^n$, we get, for all $N \in \mathbb{N}$, that

$$\left(\sum_{i=N}^{\infty} |\nu_i^n|^m\right)^{1/m} \leq K_\infty \left(\sum_{i=N}^{\infty} (E_i^n)^{-\gamma}\right)^{1/\gamma} .$$

Next we find $N \in \mathbb{N}$ large enough so that

$$||P_N(\phi_{0,\ell})||_{L^2(\Omega)} \geq 1 - \frac{1}{2}\,\varepsilon^{\gamma/m} \quad \ell = 1, 2, ...N-1\ ,$$

or, which is equivalent,

$$||Q_N(\phi_{0,\ell})||_{L^2(\Omega)} \leq \frac{1}{2}\,\varepsilon^{\gamma/m}, \quad \ell = 1, 2, ...N-1\ .$$

Then, there is $n_0 \in \mathbb{N}$ large enough so that,

$$\sum_{i=N}^{\infty} (\alpha_{i,\ell}^n)^2 \leq \varepsilon^{\gamma/m} \quad \forall\, n \geq n_0\,,\ \ell = 1, 2, ..., N-1\ .$$

Using $E_i^n = \sum_{\ell=1}^{\infty} \lambda_{0,\ell}\,(\alpha_{i,\ell}^n)^2$ and $\sum_{\ell=1}^{\infty} (\alpha_{i,\ell}^n)^2 = 1$, by concavity of $s \mapsto s^{-\gamma}$ we have

$$(E_i^n)^{-\gamma} \leq \sum_{\ell=1}^{\infty} (\alpha_{i,\ell}^n)^2\,(\lambda_{0,\ell})^{-\gamma}.$$

Hence, collecting the above estimates, we obtain

$$\begin{aligned}
\sum_{i=N}^{\infty}(E_i^n)^{-\gamma} \leq \sum_{i=N}^{\infty}\sum_{\ell=1}^{\infty}(\alpha_{i,\ell}^n)^2\,(\lambda_{0,\ell})^{-\gamma} &= \sum_{\ell=1}^{M-1}\sum_{i=N}^{\infty} \cdots + \sum_{\ell=M}^{\infty}\sum_{i=N}^{\infty} \cdots \\
&\leq \frac{M-1}{\lambda_1^{\gamma}} \sum_{i=N}^{\infty} (\alpha_{i,\ell}^n)^2 + \sum_{l=M}^{\infty} \frac{\varepsilon^{\gamma/m}}{\lambda_{0,l}^{\gamma}} \\
&\leq c\,\varepsilon^{\gamma/m}\,,
\end{aligned}$$

for some constant $c > 0$. This completes the proof of Claim (4.14).

Since $\{\|L_n\|_1\}_{n\in\mathbb{N}}$ is uniformly bounded with respect to $n \in \mathbb{N}$,

$$\sum_{i\in\mathbb{N}} |\bar{\nu}_i| < \infty\ .$$

For any $\eta \in \mathrm{L}^2(\Omega)$, by the Cauchy-Schwartz and the triangle inequality,

$$\left\| \sum_{i\in\mathbb{N}} \left(\eta,\, \bar{\psi}_i\right)_{\mathrm{L}^2(\Omega)}\ \bar{\nu}_i\, \bar{\psi}_i \right\|_{L^2(\Omega)} \leq ||\eta||_{L^2(\Omega)} \sum_{i\in\mathbb{N}} |\bar{\nu}_i| < \infty\ .$$

Hence the operator defined through

$$(\bar{L}\eta)(x) = \sum_{i\in\mathbb{N}} \left(\eta,\, \bar{\psi}_i\right)_{\mathrm{L}^2(\Omega)} \bar{\nu}_i\, \bar{\psi}_i(x), \quad x \in \Omega\ , \quad \eta \in \mathrm{L}^2(\Omega)$$

is in $\mathcal{S}_1$. Let us prove that $\{L_n\}_{n\in\mathbb{N}}$ converges to $\bar{L}$ in $\mathcal{S}_1$. Given $N \in \mathbb{N}$, denote by $P_N^n : L^2(\Omega) \to F_N^n$ the orthogonal projection onto $F_N^n = \mathrm{span}\{\psi_i^n : 1 \le i \le N-1\}$ and by $Q_N^n = I - P_N^n$ the projection onto $(F_N^n)^\perp$:

$$\|L_n - L\|_1 \le \|(L_n - L)\, P_N\|_1 + \|L_n\, Q_N^n\|_1 + \|L Q_N\,\|_1 + \|L_n\,(Q_N^n - Q_N)\|_1\ .$$

The first term converges to zero, because of the strong convergence of the first $N-1$ eigenvalues and eigenfunctions in $\mathbb{R}$ and $\mathrm{L}^2(\Omega)$ respectively. From (4.14) we have that the second and third terms are small if $N \in \mathbb{N}$ is large enough, independent of $n \in \mathbb{N}$, since

$$\Big(\sum_{i\in\mathbb{N}} |\nu_i|^n\Big)^m \le \sum_{i\in\mathbb{N}} |\nu_i^n|^m < \varepsilon\ .$$

Using (4.5), we have that

$$\|L_n(Q_N^n - Q_N)\|_1 \le \|L_n\|_1 \cdot \|Q_N^n - Q_N\|$$

which converges to zero as $n \to \infty$, since $Q_N^n - Q_N = P_N^n - P_N$ converges to zero for the same reasons as the first term.

Proof of ii) Assume now that $\sup_{n\in\mathbb{N}} \sum_{i\in\mathbb{N}} |\nu_i^n|^m = C_1$ is finite, so that using the monotonicity of $\{|\nu_i^n|^m\}_{i\in\mathbb{N}}$, for any $m' > m$ and any $N \in \mathbb{N}$,

$$\sum_{i=N}^{\infty} |\nu_i^n|^{m'} \le (\nu_N^n)^{m'-m} \sum_{i=N}^{\infty} |\nu_i^n|^m \le |\nu_N^n|^{m'-m}\, C_1\ .$$

If $\bar{\nu}_i = 0$ for all $i \in \mathbb{N}$, then

$$\lim_{n\to\infty} \sum_{i\in\mathbb{N}} |\nu_i^n|^{m'} \le \lim_{n\to\infty} |\nu_N^n|^{m'-m}\, C_1 = 0\ .$$

From here on, taking $m' = 1$ and arguing as before we obtain that $\{L_n\}_{n\in\mathbb{N}^*}$ converges to 0 in $\mathcal{S}_1$. The general case, *i.e.* when there is $i_0 \in \mathbb{N}$ such that $|\bar{\nu}_{i_0}| > 0$, follows from similar arguments. □

To generalize Theorem 4.4, we introduce the following assumptions. From now on, let $\gamma > \gamma_d \equiv d/2$ and $m = \frac{\gamma}{\gamma+1} \in (0,1]$.

Definition 4.7. We shall say that a function $\beta : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ verifies *Conditions (C)* if and only if

a) $\beta(0) = 0$,

b) $\beta(s) = \infty$ for any $s < 0$,

c) β is m-Hölder continuous at $s = 0$, *i.e.*, for some $\delta > 0$, $\beta < 0$ on $(0, \delta)$ and

$$[\beta]_m \equiv \lim_{s\to 0} \frac{|\beta(s)|}{s^m} > 0 \quad \text{if} \quad m < 1\,, \quad \text{or} \quad [\beta]_1 = +\infty \quad \text{if} \quad m = 1\,.$$

As examples of functions satisfying Conditions (C), we have, for $s > 0$, $\beta(s) = -c_m\, s^m$ or $\beta(s) = s \log s - s$.

Corollary 4.7. *Let F be a continuous $\mathcal{C}_{-\Delta,\Omega}$-function such that $\beta(s) = F^*(-s)$, $s \in \mathbb{R}$, verifies (C). If $\{L_n\}_{n\in\mathbb{N}} \subset \mathcal{H}^1_+$ is such that $\{\mathcal{K}(L_n)\}_{n\in\mathbb{N}}$ and $\{\mathcal{E}_\beta(L_n)\}_{n\in\mathbb{N}}$ are bounded, then $\{\mathcal{E}_{\beta_m}(L_n)\}_{n\in\mathbb{N}}$ is also bounded and, up to the extraction of a subsequence, $\{L_n\}_{n\in\mathbb{N}}$ converges in $\mathcal{S}_1$.*

Proof. By convexity of β, there exists $\delta > 0$ such that $\beta(s) < 0$ for all $s \in (0, \delta)$ and

$$B = \inf_{s\in(0,\delta)} \frac{|\beta(s)|}{s^m} > 0\,.$$

On other hand, from Condition (C), a), and the boundedness of the sequences $\left\{\sum_{i\in\mathbb{N}} \nu_i^n\right\}_{n\in\mathbb{N}}$ and $\left\{\sum_{i\in\mathbb{N}} \beta(\nu_i^n)\right\}_{n\in\mathbb{N}}$, for each $\varepsilon \in (0, \delta)$, we are in position to choose $N_\varepsilon \in \mathbb{N}$ such that

$$0 < \nu_i^n < \varepsilon, \quad \forall\, i \geq N_\varepsilon + 1\,,$$

for all $n \in \mathbb{N}$. Then, for n large enough,

$$\sup_{1\leq i\leq N_\varepsilon} (\nu_i^n - 2\,\bar{\nu}_i) < 0 \quad \text{and} \quad \sup_{1\leq i\leq N_\varepsilon} \frac{|\beta(\nu_i^n)|}{(\nu_i^n)^m} < 2\,B\,,$$

so that

$$\begin{aligned}\sum_{i\in\mathbb{N}}(\nu_i^n)^m &= \sum_{i=1}^{N_\varepsilon}(\nu_i^n)^m + \sum_{i=N_\varepsilon+1}^{\infty}(\nu_i^n)^m \\ &\leq 2\sum_{i=1}^{N_\varepsilon}(\bar\nu_i)^m + 2\,B\sum_{i=N_\varepsilon+1}^{\infty}|\beta(\nu_i^n)| \\ &= 2\sum_{i=1}^{N_\varepsilon}(\bar\nu_i)^m + 2\,B\left|\sum_{i=N_\varepsilon+1}^{\infty}\beta(\nu_i^n)\right| ,\end{aligned}$$

so that $\{\sum_{i\in\mathbb{N}}(\nu_i^n)^m\}_{n\in\mathbb{N}}$ is bounded and we conclude by Theorem 4.4, ii). □

Remark 4.1. The property shown in Corollary 4.7 is an analogous at operators level of the compactness of the embedding $\mathrm{H}^1(\Omega) \hookrightarrow \mathrm{L}^2(\Omega)$.

4.4. Applications (*Aplicaciones*)

4.4.1. Minimization of the free energy functional (*Minimización del funcional de energía libre*)

Consider first the free energy functional

$$\mathcal{F}_{V,\beta}^{\lambda}(L) = \mathcal{F}_{V,\beta}(L) - \lambda\,\|L\|_1 \quad L \in \mathcal{H}^1 . \tag{4.16}$$

<u>Theorem</u> 4.5. *Let V be a potential verifying (C_ε) for some $\varepsilon \in (0,1]$ and take $\lambda < \lambda_{V,1}^{\varepsilon}$. Let F be a continuous $\mathcal{C}_{-\Delta,\Omega}$-function such that*

$$\beta(s) \equiv F^*(-s) \quad \forall\, s \in \mathbb{R} ,$$

verifies (C). Then there exists $L_0 \in \mathcal{H}^1_+$ such that

$$\mathcal{F}_{V,\beta}^{\lambda}(L_0) = \inf_{L\in\mathcal{H}^1_+} \mathcal{F}_{V,\beta}^{\lambda}(L)$$

provided one of the following conditions is satisfied:

i) *if $d = 1$, $V \in \mathrm{L}^q(\mathbb{R}^d)$, for some $q \in [1,\infty]$,*

ii) *if $d = 2$, $V \in \mathrm{L}^q(\mathbb{R}^d)$, for some $q \in]1,\infty]$,*

iii) *if* $d \geq 3$, $V \in \mathrm{L}^q(\mathbb{R}^d)$, *for some* $q \in [\frac{d}{2}, \infty]$.

Proof. By Theorem 4.5 the functional $\mathcal{F}^{\lambda}_{V,\beta}$ is bounded from below. Let $\{L_n\}_{n\in\mathbb{N}^*} \subset \mathcal{H}^1_+$ be a minimizing sequence, *i.e.*,

$$\lim_{n\longrightarrow\infty} \mathcal{F}^{\lambda}_{V,\beta}(L_n) = \inf_{L\in\mathcal{H}^1_+} \mathcal{F}^{\lambda}_{V,\beta}(L) \ .$$

According to (C_ε), the coercitivity of $\mathcal{F}^{\lambda}_{V,\beta}$ implies the boundedness of $\{\mathcal{F}^{\lambda}_{V,\beta}(L_n)\}_{n\in\mathbb{N}^*}$ so that, by Corollary 4.6, the sequences $\{\|L_n\|_1\}_{n\in\mathbb{N}^*}$, $\{K(L_n)\}_{n\in\mathbb{N}^*}$, $\{\mathcal{E}_\beta(L_n)\}_{n\in\mathbb{N}^*}$ and $\{\mathcal{P}_V(L_n)\}_{n\in\mathbb{N}}$ are bounded. Corollary 4.7 provides the existence of $L_0 \in \mathcal{S}_1$ such that, up to the extraction of a subsequence, $\{L_n\}_{n\in\mathbb{N}^*}$ converges to L_0 in $\mathcal{S}_1$ so that, in particular,

$$\lim_{n\longrightarrow\infty} \|L_n\|_1 = \|L_0\|_1 \ . \tag{4.17}$$

From Condition (C), it is clear that $L_0 \geq 0$.

In order to study the entropy term we consider the space ℓ^1 with the usual norm. Consider the set

$$\mathcal{A}_+ \equiv \{u = \{u_i\}_{i\in\mathbb{N}} \in \ell^1 : \sum_{i\in\mathbb{N}} \beta(u_i) \geq A\} \ ,$$

where $A \equiv \inf_{n\in\mathbb{N}^*} \mathcal{E}_\beta(L_n)$. Both the function $D : \mathcal{A}_+ \to \mathbb{R}$ defined by

$$D(u) \equiv \sum_{i\in\mathbb{N}} \beta(u_i), \quad \forall\ u = \{u_i\}_{i\in\mathbb{N}} \in \mathcal{A}_+ \ ,$$

and the set $\mathcal{A}_+$ are convex. Thus D is weakly semi-continuous so that

$$\liminf_{n\to\infty} D(\nu_n) \geq D(\nu_0),$$

where $\nu^n = \{\nu^n_i\}_{i\in\mathbb{N}}$ and $\nu_0 = \{\bar\nu_i\}_{i\in\mathbb{N}}$. This amounts to say that

$$\liminf_{n\to\infty} \mathcal{E}_\beta(L_n) \geq \mathcal{E}_\beta(L_0) \ . \tag{4.18}$$

Next we consider the kinetic energy term. Given a fixed $N \in \mathbb{N}$, for any $n \in \mathbb{N}^*$ we have that

$$\begin{aligned} \liminf_{n\to\infty} \sum_{i\in\mathbb{N}} \nu^n_i \int_\Omega |\nabla\psi^n_i(x)|^2\, dx \ &\geq\ \liminf_{n\to\infty} \sum_{i=1}^{N} \nu^n_i \int_\Omega |\nabla\psi^n_i(x)|^2\, dx \\ &\geq\ \sum_{i=1}^{N} \bar\nu_i \int_\Omega |\nabla\bar\psi_i(x)|^2\, dx \ . \end{aligned}$$

Since the number N is arbitrary, we get

$$\liminf_{n\to\infty} \mathcal{K}(L_n) \geq \mathcal{K}(L_0) \ , \tag{4.19}$$

whence $L_0 \in \mathcal{H}^1_+$.

As for the potential energy, we obtain

$$\lim_{n\to\infty} \mathcal{P}_V(L_n) = \mathcal{P}_V(L_0) \tag{4.20}$$

using Proposition 4.2. □

To prove the uniqueness of the minimizer and a relation with the corresponding problem at mixed sates level we need some extra information. So, let us consider the following additional condition.

Definition 4.8. We shall say that a function $\beta : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ and a potential V on Ω satisfy the condition (H) if

H1) β is a strictly convex function which is C^1 in the interior of its support;

H2) $-\Delta + V$ has an infinite sequence $\{\lambda_i(V)\}_{i\in\mathbb{N}}$ of eigenvalues diverging to ∞;

H3) the operators $\zeta(-\Delta + V)$ and $\eta(-\Delta + V)$ are in $\mathcal{S}_1$, where

$$\zeta(s) = \beta \circ (\beta')^{-1}(-s) \quad \text{and} \quad \eta(s) = -s(\beta')^{-1}(-s).$$

Notice that we have already seen several conditions ensuring that Condition (H2) is satisfied. Recall that the commutator operator is given by $[L, R] = LR - RL$. Define

$$\mathcal{F}^{\lambda}_{V,\beta}[\nu, \psi] \equiv \sum_{i\in\mathbb{N}} \left[\beta(\nu_i) + \nu_i \int_\Omega \left(|\nabla\psi_i|^2 + (V(x) - \lambda)|\psi_i|^2\right) dx\right] , \tag{4.21}$$

and denote by S the set of non-increasing sequences $\{\nu_i\}_{i\in\mathbb{N}} \subset \mathbb{R}_+$ converging to zero, such that $\sum_{i\in\mathbb{N}} \beta(\nu_i)$ is absolutely convergent. Let

$$\mathcal{X} \equiv \{(\nu, \psi) \in S \times \left(L^2(\mathbb{R}^d)\right)^{\mathbb{N}} : (\psi_i, \psi_j)_{L^2(\Omega)} = \delta_{ij}, \forall\, i, j \in \mathbb{N}\} \ .$$

Corollary 4.8. *Under the conditions of Theorem 4.5, if (V,β) verify (H), then*

$$L_\lambda = (\beta')^{-1}(-(-\Delta + V - \lambda))) \tag{4.22}$$

is the unique minimizer of $\mathcal{F}^\lambda_{V,\beta}$. The operator L_λ is a stationary solution of the Heisenberg equation

$$[-\Delta + V - \lambda,\, L_\lambda] = 0\ .$$

Additionally, a mixed state $\{\nu(L_\lambda), \psi(L_\lambda)\} = \{\nu_i(L_\lambda), \psi_i(L_\lambda)\}_{i\in\mathbb{N}}$ realizes the minimum

$$\min_{(\nu,\psi)\in\mathcal{X}} \mathcal{F}^\lambda_{V,\beta}[\nu,\psi]\ . \tag{4.23}$$

Observe that in the context of Theorem 4.5 and Corollary 4.8, Condition (H3) just means that $F \in \mathcal{C}_{-\Delta+V,\Omega}$.

Notice that mixed states are not uniquely defined, for instance if some eigenvalues have multiplicity larger than 1.

Lemma 4.3. *The minimization problem (4.23) has a solution*

$$(\bar\nu, \bar\psi) = \{(\bar\nu_i, \bar\psi_i)\}_{i\in\mathbb{N}} \in \mathcal{X},$$

which is unique up to any unitary transformation, which leaves all eigenspaces of $-\Delta + V - \lambda$ invariant. Additionaly, for every $i \in \mathbb{N}$ it verifies

$$\begin{cases} \bar\nu_i = (\beta')^{-1}(\lambda - \lambda_i(V)), \\ \bar\psi_i \in \mathrm{H}^1_0(\Omega). \end{cases} \tag{4.24}$$

The proof is quite similar to the one of [26, Proposition 4] in $\mathbb{R}^d$ in the case of a non-negative potential V and for $\lambda = 0$. The main idea is to work with finite sums first and pass to the limit afterwards. We refer to [26] for more details.

Proof (Corollary 4.8). We have that

$$\mathcal{F}^\lambda_{V,\beta}(L_\lambda) = \mathcal{F}^\lambda_{V,\beta}[\nu(L_\lambda), \psi(L_\lambda)] = \inf\{\mathcal{F}^\lambda_{V,\beta}[\nu(R), \psi(R)] :\ R \in \mathcal{H}^1_+\}\ . \tag{4.25}$$

Reciprocally, to $(\bar\nu, \bar\psi) \equiv \{(\bar\nu_i, \bar\psi_i)\}_{i\in\mathbb{N}} \in \mathcal{X}$, we can associate

$$\bar L\eta = \sum_{i\in\mathbb{N}} \bar\nu_i \left(\eta,\, \bar\psi_i\right)_{\mathrm{L}^2(\Omega)} \bar\psi_i \quad \forall\, \eta \in \mathrm{L}^2(\mathbb{R}^d)\ . \tag{4.26}$$

Assume that $(\bar\nu, \bar\psi)$ realizes the minimum of $F^\lambda_{V,\beta}[\nu,\psi]$. Since $\bar L \in \mathcal{H}^1_+$ is not affected by any unitary transformation leaving all eigenspaces of $-\Delta + V - \lambda$ invariant, $\bar L = L_\lambda$ and L_λ is unique. □

4.4.2. Free energy involving a non-linear but local function of the density function (*Energía libre con una no-linearidad que es función local de la densidad*)

Consider the free energy functional given by

$$\mathcal{F}^{\lambda,g}_{V,\beta}(L) \equiv \mathcal{F}^{\lambda}_{V,\beta} + \mathcal{G}(L) \quad \forall\, L \in \mathcal{H}^1 \ ,$$

where

$$\mathcal{G}(L) = \int_{\Omega} g(\rho_L(x))\, dx$$

and g is some real function, which is not necessarily convex. Using the machinery presented in Section 4.4.1, we obtain the following result.

<u>**Theorem**</u> **4.6.** *Let V be a potential on Ω verifying (C_ε), for some $\varepsilon \in (0,1]$. Let $\lambda < \lambda^{\varepsilon}_{V,1}$ and assume that $F \in \mathcal{C}_{-\Delta,\Omega}$ is such that $\beta(s) \equiv F^*(-s)$ verifies (C). Let $g \in \mathrm{C}([0,\infty))$ be bounded from below and such that*

$$|g(s)| \leq s^q \quad \forall\, s \geq s_0 \ , \tag{4.27}$$

for some $s_0 \geq 0$, where

- ***i)*** *$q \in [1,\infty)$ if $d = 1$ or $d = 2$,*
- ***ii)*** *$q \in [1, d/(d-2)]$ if $d \geq 3$.*

Then there exists $L_\infty \in \mathcal{H}^1_+$ such that

$$\mathcal{F}^{\lambda,g}_{V,\beta}(L_\infty) = \inf_{L \in \mathcal{H}^1_+} \mathcal{F}^{\lambda,g}_{V,\beta}(L) \ .$$

Moreover, if $g \in \mathrm{C}^1([0,\infty))$, L_∞ is a fixed point of the application $Y : \mathcal{H}^1_+ \longrightarrow \mathcal{H}^1_+$ given by

$$Y(L) = (\beta')^{-1}\left(-(-\Delta + V) + \lambda - g' \circ \rho_L\right).$$

Demostración. It is similar to the one of Theorem 4.5. We use condition (4.27) to show via Fatou's lemma that

$$\mathcal{G}(L_\infty) \leq \liminf_{n \longrightarrow \infty} \mathcal{G}(L_n) \ ,$$

where $\{L_n\}_{n\in\mathbb{N}} \subset \mathcal{H}^1_+$ is a minimizing sequence for $\mathcal{F}^{\lambda,g}_{V,\beta}$. □

4.4.3. Stationary states for the Hartree problem with temperature (*Estados estacionarios para el problema de Hartree con temperatura*)

Consider a Heisenberg equation with a Poisson coupling, namely

$$\begin{cases} i\,\partial_t L(t) = [-\Delta + V(t,\cdot), L(t)] & t \geq 0 \, , \\ -\Delta V(t,x) = \rho_{L(t)}(x) & x \in \Omega \, , \quad t \geq 0 \, , \\ L(0) = \tilde{L} \end{cases} \tag{4.28}$$

where $L(t)$, the *density operator of the system*, is a positive trace-class operator acting on $\mathrm{L}^2(\Omega)$ and $[L,R] = LR - RL$.

We assume $d \leq 4$ and restrict our study to the case of homogeneous Dirichlet boundary conditions:

$$V = 0 \quad \text{on } \partial\Omega \, .$$

The stationary states of (4.28) are then solutions of

$$\begin{cases} [-\Delta + V, L] = 0 \, , \\ -\Delta V = \rho_L \, . \end{cases} \tag{4.29}$$

Let $F \in \mathcal{C}_{-\Delta,\Omega}$ a non-negative function of class C^1 such that $F' \in \mathcal{C}_{-\Delta,\Omega}$. Then if $(L_F, V_F) \in \mathcal{H}^1 \times \mathrm{H}^1_0(\Omega)$ is solution of

$$\begin{cases} -\Delta V = \rho_L & \text{in } \Omega \, , \\ L = -F'(-\Delta + V) \end{cases} \tag{4.30}$$

it holds that

$$[-\Delta + V_F, L_F] = 0 \, ,$$

so that (L_F, V_F) is a solution for (4.29).

Stationary states of (4.28) are obtained through the minimization of the free energy

$$\mathcal{F}_\beta(L) = \mathcal{E}_\beta(L) + \mathcal{K}(L) + \mathcal{P}(L), \quad \forall\, L \in \mathcal{H} \, ,$$

where

$$\mathcal{P}(L) = \frac{1}{2}\int_\Omega V_L \rho_L \, dx = \frac{1}{2}\int_\Omega |\nabla V_L|^2 \, dx \, .$$

Theorem 4.7. *Let F be a continuous $\mathcal{C}_{-\Delta,\Omega}$-function such that*

$$\beta(s) \equiv F^*(-s), \quad \forall s \in \mathbb{R},$$

verifies (C). Then there exists $L_F \in \mathcal{H}^1_+$ such that

$$\mathcal{F}_\beta(L_F) \le \mathcal{F}_\beta(L), \qquad \forall\, L \in \mathcal{H}^1. \tag{4.31}$$

Moreover if β verifies (H1), i.e. if it's C^1 in the interior of its support, then

$$L_F = (\beta')^{-1}(-(-\Delta + V_{L_F}))$$

is the unique minimizer of $\mathcal{F}_\beta$ and solves (4.29) as well.

Proof. The proof is almost a copy of the one of Theorem 4.5. The argument changes minimally to reach $\text{lím}_{n\to\infty} \mathcal{P}(L_n) = \mathcal{P}(L_F)$, but it still depends on Proposition 4.2. □

The case with an attracting Poisson coupling, *i.e.*,

$$+\Delta V = \rho_L \quad \text{in } \Omega\ ,$$

can be dealt with the same methods although it makes less sense from the point of view of physics. Some additional work is necessary to establish spectral properties of $-\Delta + V_L$.

As a concluding remark, let us notice that if β is non-negative then the minimizer in Theorem 4.7 is $L_F = 0$. However, the result applies to functions β for which $\{\beta < 0\} \neq \emptyset$ as it is the case for

$$\beta(s) = \begin{cases} s \log s - s & \text{if } s > 0\ , \\ 0 & \text{if } s = 0\ , \\ +\infty & \text{if } s < 0\ . \end{cases}$$

For stationary states having a prescribed total charge we have got a generalization of [60, Theorem 2] at operators level. Mathematically, the free energy is changed only by a term $-\lambda \int_\Omega \rho_L\, dx$, where λ is the Lagrange multiplier associated to the mass constraint. The generating function β of the entropy term is now changed into $\nu \mapsto \beta(\nu) - \lambda\,\nu$, which results in the fact that the set $\{\nu \in \mathbb{R} : \nu \mapsto \beta(\nu) - \lambda\,\nu < 0\}$ is automatically non-empty. Because of the compactness property, the mass constraint will be verified when passing to the limit in a minimizing sequence.

Moreover, with almost no work, we can add an external potential which has a non-zero negative component and eventually singularities of, for instance, Coulomb type. This situation is highly relevant from a physics point of view, for the modelization of atomic and molecular systems, without temperature, see for instance [70] and references therein, or with temperature, see [59]. In such a case, the appropriate model is rather the Hartree-Fock system than the the Hartree system.

4.5. A Quantum Drift-Diffusion problem (*Un problema de* Quantum Drift-Diffusion)

Now we bring our attention to the problem which motivated the research presented in Sections 4.1-4.4.

4.5.1. The problem (*El problema*)

Let $d \in \mathbb{N}$ and $\Omega \subset \mathbb{R}^d$ a bounded domain with boundary $\partial\Omega$ of class C^1. In [31] we consider the following Quantum Drift-Diffusion (QDD) model

$$\begin{cases} \partial_t \rho(t,x) + \operatorname{div}\left(\rho(t,x)\nabla A(t,x)\right) = 0, & (t,x) \in]0,\infty[\times\Omega, \\ L(t) = \exp\left(-(-h^2\Delta + A(t) + V)\right), & t \in]0,\infty[, \end{cases} \tag{4.32}$$

where V is a given potential on Ω and, for each $t \in]0,\infty[$, $L(t)$ is a positive selfadjoint trace-class operator whose associated density, $\rho(t)$, is given by

$$\rho(t,x) = \sum_{i\in\mathbb{N}} \nu_i(t)|\psi_i(t,x)|^2, \quad t > 0,\ x \in \Omega.$$

Here $\{\nu_i(t)\}_{i\in\mathbb{N}} \subset \mathbb{R}_+$ is the sequence of eigenvalues of $L(t)$ and $\{\psi(t,\cdot)\}_{i\in\mathbb{N}}$ is the corresponding $\mathrm{L}^2(\Omega)$-complete orthonormal sequence of eigenstates. If we denote by $\{\lambda_i(t)\}_{i\in\mathbb{N}}$ the sequence of eigenvalues of $-\Delta + A(t) + V$, then

$$\nu_i(t) = \exp(-\lambda_i(t)), \quad \forall i \in \mathbb{N}.$$

We assume that for some $A_0 \in \mathrm{L}^2(\Omega)$, it verifies

$$\begin{cases} A(0) = A_0, \\ L(0) = L_0 \equiv \exp(-(-h^2\Delta + A_0 + U)). \end{cases}$$

To find a solution for (4.32) our machinery works as follows. The interval $[0, \infty)$ is discretized as $t_k = k\tau$, where $k \in \mathbb{N}^*$ and $\tau > 0$. At each step, it is found a minimizer $L_{\tau,k+1}$ of the *step functional* which results of adding to an appropiate free energy functional the Wasserstein distance beetwen the densities associated respectively to the argument L and to the operator obtained in the previous step, $L_{\tau,k}$. Then we interpolate: $L_\tau(t) = L_{\tau,k}$, for $(t, k) \in [k\tau, (k+1)\tau) \times \mathbb{N}$, and pass to the limit as $\tau \longrightarrow 0$. The kind of semidiscretization just mentioned has its origin in [49].

The QDD model was derived in [19], [21] and [20] using Levermore's methodology, based on an entropy minimization. Roughly speaking, the goal was to stablish the relations beetwen the macroscopic and microscopic descriptions of large particle quantum systems (e.g. semiconductors and some types of plasmas). The objective was to obtain a new macroscopic transport model taking account of the efects of quantum collisions at a diffusive scale.

A version of the QDD problem at mixed states level was numerically treated in [39] (see also [38]) where, in addition, it was assumed that the density ρ and a self-consistent potential V_{aut} are linked by

$$\begin{cases} -\Delta V_{\text{aut}} = \rho, & \text{in} \quad \Omega; \\ \quad V_{\text{aut}} = 0, & \text{on} \quad \partial\Omega \end{cases}$$

The semidiscretization used by the authors is quite natural, a finite differences scheme, and presents good properties e.g it preserves the positivity of the density and the total charge, and it is such that the free energy dissipates. However the convergence to the original problem is not an easy task. This guided us to consider a version of (4.32) at mixed states level whose derivation uses ideas taken from [28, Section 5]. To prove the validity of the last there are stability difficulties in the minimization process which made us consider a machinery at operators level instead of the mixed states setting.

4.5.2. The Wasserstein metric (*La métrica de Wasserstein*)

Let's equip the set of densities

$$\mathcal{N}(\Omega) = \{f \in \mathrm{L}^1(\Omega) : \; f \geq 0, \text{ a.e. } \Omega, \text{ and } ||f||_{L^1(\Omega)} = 1\}, \tag{4.33}$$

with the Wasserstein metric, $W(\cdot,\cdot)$, given by an optimal mass transference problem:

$$W^2(n,m) \equiv \inf_{\gamma\in\Pi(n,m)} \int_{\Omega\times\Omega} |x-y|^2\gamma(dx,dy) \tag{4.34}$$

where the cost function is $c(x,y) = |x-y|^2$ and $\Pi(n,m)$ is the set of all couplings of n and m, i.e., all the probability measures γ on $\Omega\times\Omega$ such that for every $\psi \in C_0^\infty(\Omega)$ it verifies

$$\begin{aligned}\int_{\Omega\times\Omega} \psi(x)\gamma(dx,dy) &= \int_\Omega \psi(x)n(x)dx,\\ \int_{\Omega\times\Omega} \psi(y)\gamma(dx,dy) &= \int_\Omega \psi(y)m(y)dy.\end{aligned}$$

The problem (4.34) has a unique minimizer $\gamma_{n,m} \in \Pi(n,m)$. Moreover, there exists a convex function $\phi = \phi_{m,n}$ whose gradient provides the optimal transference plan for $m(x)dx$ and $n(x)dx$, i.e. it verifies

$$W^2(n,m) = \int_\Omega |x-\nabla\phi(x)|^2 m(x)dx. \tag{4.35}$$

The last is denoted by $n = \nabla\phi\#m$ and corresponds to the validity of the relation

$$\int_\Omega \psi(y)n(y)dy = \int_\Omega \psi(\nabla\phi(x))m(x)dx, \quad \forall\psi\in C_0^\infty(\Omega). \tag{4.36}$$

Remark 4.2. The function ϕ and its Fenchel transform ϕ^* are differentiable up to a set of $d-1$-Hausdorff dimension. It also holds

$$\nabla\phi(\nabla\phi^*(w)) = w, \qquad n(w)dw - a.e.\ w\in\Omega,$$

$$\nabla\phi^*(\nabla\phi(w)) = w, \qquad m(w)dw - a.e.\ w\in\Omega.$$

Finally, if $m \in \mathcal{N}(\Omega)$ is fixed, then the derivative of $W^2(\cdot,m)$ is given by

$$\langle D_n W^2(n,m),\tilde n\rangle = 2\int_\Omega \left(\frac{|y|^2}{2} - \phi^*(y)\right)\tilde n(y)dy, \quad \forall\tilde n\in\mathcal{N}(\Omega). \tag{4.37}$$

For a detailed exposition on optimal mass transference problems (in particular the Wasserstein metric) we refer to [74], [13] and [2].

4.5.3. The step problem (*El problema de paso*)

Let's consider the following Nehari-type subset of $\mathcal{H}^1_+$:

$$\mathcal{N}^1 = \{L \in \mathcal{H}^1_+ : \|L\|_1 = 1\}.$$

The following result says that the set of operators in $\mathcal{N}^1$ having finite entropy is arcwise connected

Proposition 4.6. *Let $F \in \mathcal{C}_{-\Delta,\Omega}$. Let L_0, $L_1 \in \mathcal{N}^1$ be such that $\mathcal{E}_\beta(L_0)$ and $\mathcal{E}_\beta(L_1)$ are finite. Here $\beta(s) = F^*(-s)$. Then there exists a curve $\gamma : [0,1] \longrightarrow \mathcal{N}^1$ of class C^1 such that $\gamma(0) = L_0$ and $\gamma(1) = L_1$.*

Sketch of the proof. Let's denote by $\{(\nu_k(0), \psi_k(0))\}_{k\in\mathbb{N}}$ and $\{(\nu_k(0), \psi_k(0))\}_{k\in\mathbb{N}}$ the mixed states associated to L_0 and L_1 respectively. For $N \in \mathbb{N}$ and $\eta \in \mathrm{L}^2(\Omega)$ we put

$$L_0^{(N)}\eta = \sum_{k=1}^{N} \left(\frac{\nu_k(0)}{\sum_{j=1}^{N} \nu_j(0)} \right) (\eta,\, \psi_k(0))_{\mathrm{L}^2(\Omega)}\, \psi_k(0),$$

and

$$L_1^{(N)}\eta = \sum_{k=1}^{N} \left(\frac{\nu_k(1)}{\sum_{j=1}^{N} \nu_j(1)} \right) (\eta,\, \psi_k(1))_{\mathrm{L}^2(\Omega)}\, \psi_k(1),$$

so that the operators $L_0^{(N)}$ and $L_1^{(N)}$ are of finite rank and live in $\mathcal{N}^1$.

We take a selfadjoint operator σ_N on $\mathrm{L}^2(\Omega)$ such that $e^{i\sigma_N} L_0^{(N)} = L_1^{(N)}$. Then, for $\alpha \in (0,1)$ and $k \in \mathbb{N}$ we put

$$\nu_k^{(N)}(\alpha) = \alpha\nu_k^{(N)}(1) + (1-\alpha)\nu_k^{(N)}(0),$$

where

$$\nu_k^{(N)}(0) = \frac{\nu_k(0)}{\sum_{j=1}^{N} \nu_j(0)}$$

and

$$\nu_k^{(N)}(1) = \frac{\nu_k(1)}{\sum_{j=1}^{N} \nu_j(1)}$$

are the eigenvalues of $L_0^{(N)}$ and $L_1^{(N)}$ respectively. We also write

$$\psi_k^{(N)}(\alpha) = e^{i\alpha\sigma_N}\psi_k(0), \quad k \in \mathbb{N},$$

and define an operator $\gamma^{(N)}(\alpha)$ on $\mathrm{L}^2(\Omega)$ by

$$\gamma^{(N)}(\alpha)\eta = \sum_{k=1}^{N} \nu_k^{(N)} \left(\eta,\, \psi_k^{(N)}(\alpha)\right)_{\mathrm{L}^2(\Omega)} \psi_k^{(N)}(\alpha).$$

It's clear that $\left\{\psi_k^{(N)}(\alpha)\right\}_{k=1}^{N}$ is orthonormal in $\mathrm{L}^2(\Omega)$.

For each $k = 1, ..., N$, we have that $\psi_k^{(N)}(\alpha) \in \mathrm{H}_0^1(\Omega)$. Then $\gamma^{(N)}(\alpha)$ is a finite rank operator living in $\mathcal{N}^1$. Moreover, since $\mathcal{E}_\beta(L_0)$ and $\mathcal{E}_\beta(L_1)$ are finite, the sequence $\{\mathcal{E}_\beta(\gamma^{(N)}(\alpha))\}_{N\in\mathbb{N}}$ is bounded. Therefore, by the Corollary 4.7, there exists $\gamma(\alpha) \in \mathcal{S}_1$ such that $\gamma^{(N)}(\alpha) \longrightarrow \gamma(\alpha)$, as $N \longrightarrow \infty$, in $\mathcal{I}_1$. It's clear that $\gamma(\alpha) \geq 0$ and that $\|\gamma(\alpha)\|_1 = 1$.

Because of the construction we used it follows that $\gamma(\alpha) \in \mathcal{H}_+^1$ so that actually $\gamma(\alpha) \in \mathcal{N}^1$. □

Let $L_{\tau,k} \in \mathcal{N}^1$ be fixed. We define a functional on $\mathcal{N}^1$ by

$$\mathcal{W}(L) \equiv \frac{1}{2} W^2(\rho_L,\, \rho_{\tau,k}), \tag{4.38}$$

where $\rho_{\tau,k}$ is the density function associated to $L_{\tau,k}$ and $\rho_L = \nabla\phi_L \# \rho_{\tau,k}$. We have the following

Theorem 4.8. *Let $\tau > 0$. Let V be a potential on Ω which verifies (C_ε), for some $\varepsilon \in (0, 1]$. Let $\lambda < \lambda_{V,1}^{\varepsilon}$ and $F \in \mathcal{C}_{-\Delta,\Omega}$ be continuous and such that $\beta(s) \equiv F^*(-s)$ verifies (C). Then there exists an operator $L_{\tau,k+1} \in \mathcal{N}^1$ such that*

$$\mathcal{I}(L_{\tau,k+1}) = \inf_{L\in\mathcal{N}^1} \mathcal{I}(L),$$

where

$$\mathcal{I}(L) = \frac{1}{\tau}\mathcal{W}(L) + \mathcal{F}_{V,\beta}^{\lambda}, \quad L \in \mathcal{N}^1.$$

Moreover,

$$L_{\tau,k+1} = (\beta')^{-1} \left[\lambda_{\tau,k+1} - (-\Delta + A_{\tau,k+1} + V)\right], \tag{4.39}$$

where

$$A_{\tau,k+1}(x) \equiv \frac{1}{\tau}\left(\frac{|x|^2}{2} - \phi_{L_{\tau,k+1}}^*(x)\right), \quad x \in \Omega.$$

Proof. We follow the steps as in the proof of Theorem 4.5. Let's just show that

$$\mathcal{W}(L_{\tau,k+1}) \leq \liminf_{n\longrightarrow\infty} \mathcal{W}(L_n).$$

For each $n \in \mathbb{N}$ we choose $\gamma_n \in \Pi(\rho_n, \rho_{\tau,k})$ such that

$$\int_{\Omega\times\Omega} |x-y|^2 \gamma_n(dx,dy) \leq W^2(\rho_n, \rho_{\tau,k}) + \frac{1}{n}.$$

Since

$$\rho_n \longrightarrow \rho_{\tau,k+1}, \quad \text{as } n \longrightarrow \infty, \text{ in } \mathrm{L}^1(\mathbb{R}^d),$$

where

$$\rho_{\tau,k+1} = \rho_{L_{\tau,k+1}},$$

it is clear that $(\rho_n(x)dx)_{n\in\mathbb{N}}$ weakly converges to $\rho_{\tau,k+1}(x)dx$. Then $(\gamma_n)_{n\in\mathbb{N}}$ is *tight*, that is, up to subsequences, $(\gamma_n)_{n\in\mathbb{N}}$ weakly converges to some $\gamma \in \Pi(\rho_{\tau,k+1}, \rho_{\tau,k})$. Therefore,

$$\begin{aligned} W^2(\rho_{\tau,k+1}, \rho_{\tau,k}) &\leq \int_{\Omega\times\Omega} |x-y|^2 \gamma(dx,dy) \\ &\leq \lim_{n\longrightarrow\infty} \int_{\Omega\times\Omega} |x-y|^2 \gamma_n(dx,dy) \\ &\leq \liminf_{n\longrightarrow\infty} W^2(\rho_n, \rho_{\tau,k}). \end{aligned}$$

□

Capítulo 5

Conclusiones

5.1. Sobre el Capítulo 3

En el Capítulo 3 se considera el problema

$$\begin{cases} \varepsilon^2 \Delta v - V(x)v + |v|^{p-1}v = 0, & \text{in} \quad \mathbb{R}^d; \\ v(x) \to 0, & \text{as} \quad |x| \longrightarrow \infty \end{cases}, \tag{P_ε}$$

donde el interior del conjunto de zeros del potencial V es un abierto no-vacío. Recientemente en [11, 12] Byeon y Wang, trataron este problema, que en su contexto es referido como *flat case*. Encuentran una familia de soluciones positivas $\{v_\varepsilon\}_{\varepsilon>0}$ cuyo comportamiento contrasta al del caso $\inf V > 0$ (que ha recibido gran atención en el último tiempo). Por ejemplo, muestran que en el límite semi-clásico, i.e. cuando $\varepsilon \longrightarrow 0$, la amplitud de v_ε se va a cero, es decir,

$$\liminf_{\varepsilon \to 0} \max_{x \in \mathbb{R}^N} |v_\varepsilon(x)| = 0. \tag{5.1}$$

Para el flat case el problema límite es

$$\begin{cases} \Delta u + |u|^{p-1}u = 0, & \text{in} \quad \Omega; \\ u = 0, & \text{on} \quad \partial\Omega \end{cases} \tag{P}$$

Las soluciones $\{v_\varepsilon\}_{\varepsilon>0}$ encontradas por Byeon y Wang son de mínima energía o ground states y convergen, módulo reescalamiento, a soluciones de mínima energía de (P). Prueban además que las soluciones v_ε decaen exponencialmente a cero por fuera Ω.

Al detenernos en el problema límite nos damos cuenta que a la par de las soluciones de mínima energía hay también muchas otras soluciones. De hecho una aplicación de la teoría de Ljusternik-Schnirelman (para funcionales pares) provée la existencia de infinitas soluciones. La pregunta natural es entonces *¿Tiene el problema (P_ε) infinitas soluciones y qué relacion las liga a las soluciones de (P)*?

Damos respuesta a esta pregunta en el

Teorema 5.1. *Bajo las hipótesis generales (V1), (V2) y (V3), y asumiendo que $d \geq 3$ y que $1 < p < (d+2)/(d-2)$, se tiene que*

i) *dado $\varepsilon > 0$, el funcional J_ε tiene un número infinito de puntos críticos $\{\hat{w}_{k,\varepsilon}\}_{k\in\mathbb{N}} \subset \mathcal{M}_\varepsilon$;*

ii) *el funcional límite J tiene un número infinito de puntos críticos $\{\hat{w}_k\}_{k\in\mathbb{N}} \subset \mathcal{M}$;*

iii) *dado $k \in \mathbb{N}$, los valores críticos verifican*

$$\lim_{\varepsilon\to 0} J_\varepsilon(\hat{w}_{k,\varepsilon}) = J(\hat{w}_k); \tag{5.2}$$

iv) *más aún, dado $\delta, c > 0$, existe $\varepsilon_0 > 0$ tal que*

$$|\hat{w}_{k,\varepsilon}(x)| < C \cdot \exp\{-\frac{c}{\varepsilon} \cdot \mathrm{dist}(x, \Omega^\delta)\}, \quad \forall x \in \mathbb{R}^d,\ \forall \varepsilon \in]0, \varepsilon_0), \tag{5.3}$$

donde $C > 0$ y $\Omega^\delta = \{x \in \mathbb{R}^d : \mathrm{dist}(x, \Omega) < \delta\}$;

v) *sobre la frontera de Ω, las funciones $\hat{w}_{k,\varepsilon}$ verifican*

$$\lim_{\varepsilon\to 0} \max_{x\in\partial\Omega} |\hat{w}_{k,\varepsilon}(x)| = 0, \quad \forall k \in \mathbb{N}. \tag{5.4}$$

Se prueba que el problema (P_ε) tiene infinitas soluciones del tipo Ljusternik-Schnirelman cuyos niveles críticos convergen a los del problema (P). Probamos que estas soluciones presentan el mismo tipo de comportamiento de la solución de mínima energía encontrada por Byeon y Wang lo que parecería indicar que esta es una característica del flat case. Por otra parte, mencionemos que no sólo obtenemos decaimiento exponencial de las soluciones por fuera de Ω sino que en el punto v) del Teorema 3.1 también se presentan estimaciones asintóticas respecto al comportamiento sobre la frontera del dominio.

No se afirma nada respecto al signo de las soluciones encontradas. Sin embargo, puesto que el problema límite (P) puede tener muchas soluciones positivas dependiendo de la geometría de Ω (véase e.g. [17]), lo mismo podría suceder con (P_ε).

Obsérvese que se considera sólo el caso en que el potencial V diverge cuando $|x| \to \infty$, y cuyo conjunto de ceros es un abierto, conexo con frontera suave. Pensamos que nuestros resultados siguen teniendo validez cuando se consideran potenciales más generales, cuando Ω no es conexo, y también para los caso *finito* e *infinito* tratados en [11]. Particularmente interesante es el caso de un potencial positivo al infinito. En este caso, la existencia de infinitos puntos críticos, como en el punto i) del Teorema 3.1, podría dejar de ser cierto. Sin embargo, los puntos ii)-v), con k fija, deberían ser ciertos.

5.2. Sobre el Capítulo 4

La investigación presentada en el Capítulo 4 fue motivada básicamente por dos trabajos recientes: [26] y [31]. El primero trata con desigualdades tipo Lieb-Thirring y en el segundo se estudia un modelo de *Quantum Drift-Diffusion* como un descenso veloz de un funcional de energía libre con respecto a la métrica de Wasserstein.

En el caso de sistemas ortonormales y sub-ortonormales, desigualdades de interpolación tipo Gagliardo-Niremberg provéen información sobre constantes óptimas en desigualdades tipo traza (véase [57, 56, 40, 32]), que pueden ser extendidas a desigualdades tipo Lieb-Thirring (véase[55, 26]).
Inversamente, el conocimiento de desigualdades tipo Lieb-Thirring puede ser traducido a desigualdades de interpolación para *estados mixtos* que son sistemas infinitos de funciones ortogonales con números de ocupación (véase [26]).

En nuestra investigación reescribimos y extendemos estas desigualdades de interpolación en términos de operadores de traza autoadjuntos. Fijamos nuestra atención en el caso $\Omega \subset \mathbb{R}^d$. Luego estudiamos, a nivel de operadores, las propiedades de compacidad de las correspondientes inmersiones; estas extienden las bien conocidas propiedades de las inmersiones de Sobolev.

Dado un potencial, la minimización del funcional de energía libre es equivalente a probar desigualdades de Lieb-Thirring. Por otro lado, cuando se optimiza sobre el potencial se recuperan desigualdades de interpolación.

El primer paso que damos es acotar por debajo el funcional de energía libre, *i.e.* establecer una adaptación de las desigualdades tipo Lieb-Thirring. Como segundo paso, reformulamos estas desigualdades en términos de desigualdades de interpolación del tipo Gagliardo-Nirenberg y entonces estudiamos las propiedades de compacidad. El proceso de minimización se vuelve más o menos trivial, proveyendo casi gratuitamente la existencia de minimizadores incluso para el caso del acoplamiento de Poisson. Lo dicho corresponde al siguiente

Teorema 5.2. *Sea $\varepsilon \in (0,1)$. Supongamos que para un potencial dado, $V = V(x)$, el operador $-(1-\varepsilon)\,\Delta + V$ está acotado inferiormente por alguna constante λ. Sean F y G tales que para alguna función no-negativa f que verifica $\int_0^\infty f(t)\,\big(1+t^{-d/2}\big)\,t^{-1}\,dt < \infty$,*

$$F(s) := \int_0^\infty e^{-t\,s}\,f(t)\,\frac{dt}{t} \quad \textit{and} \quad G(s) := \int_0^\infty e^{-t\,s}\,(4\pi\,t)^{-d/2}\,f(t)\,\frac{dt}{t}\,,$$

y $\beta(s) \equiv F^*(-s)$. Entonces, para todo operador de traza L, no-negativo y autoadjunto,

$$\mathrm{Tr}\,[\beta(L) + (-\Delta + V - \lambda)\,L] \geq -\mathrm{Tr}\,\big[F\big(-\Delta + V - \lambda\big)\big]\,. \tag{5.5}$$

Si W es una perturbación no-negativa de V, se tiene que

$$\mathrm{Tr}\,[\beta(L) + (-\Delta + V + W - \lambda)\,L] \geq -\varepsilon^{-d/2}\int_\Omega G(W)\,dx\,. \tag{5.6}$$

Más aun si τ es una función tal que $G(s) = \tau^*(-s)$,

$$\mathrm{Tr}\,[\beta(L) + (-\Delta + V - \lambda)L] \geq \varepsilon^{-d/2}\int_\Omega \big(\varepsilon^{d/2}\rho_L(x)\big)\,dx.$$

Adicionalmente, si $\{L_n\}_{n\in\mathbb{N}^*}$ es una sucesión de operadores de traza no-negativos y autoadjuntos, tal que

$$\{\mathrm{Tr}\,[\beta(L_n) + (-\Delta + V - \lambda)\,L_n]\}_{n\in\mathbb{N}^*}$$

está acotada, entonces $\{L_n\}_{n\in\mathbb{N}^*}$ es relativamente compacta y converge, módulo subsucesiones, a algún $L \in \mathcal{S}_1$. Finalmente, ρ_{L_n} converge a ρ_L en $L^q(\Omega)$, para todo $q \in [1,\infty)$ si $d = 1,2$ y $q \in [1, d/(d-2)]$ si $d \geq 3$.

Con esta maquinaria en mano, es inmediata la resolución del *problema de paso* en el método usado en [31] para un modelo de Quantum Drift-Diffusion. En particular, esta minimización provée la estructura de la segunda ecuación en el sistema

$$\begin{cases} \partial_t \rho(t,x) + \operatorname{div}\left(\rho(t,x)\nabla A(t,x)\right) = 0, & (t,x) \in]0,\infty[\times\Omega, \\ L(t) = \exp\left(-(-h^2\Delta + A(t) + V)\right), & t \in]0,\infty[, \end{cases} \tag{5.7}$$

Para la ecuación diferencial, es clave el resultado de conexidad por arcos para subconjuntos de $\mathcal{N}^1 = \{L \in \mathcal{H}^1_+ : \|L\|_1 = 1\}$ cuyos elementos tienen entropía finita pues permite trabajar con perturbaciones a nivel de operadores L a la par de perturbaciones para las correspondientes funciones de densidad ρ_L. Este trabajo está en desarrollo.

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