Asymptotics of the Ground State Energies of Large Coulomb Systems*

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Abstract

We prove the Scott conjecture for molecules.

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1. Introduction and Result

Consider a molecule consisting of N electrons, each of the charge -1 and M nuclei of charges $Z_1, \ldots, Z_M$. The position and spin space of a single electron are ^{3} and $_2$, respectively. We assume that the system is neutral, i.e.

$$N = \sum_{i=1}^{M} Z_i \ ,$$

and that the nuclei are infinitely heavy and located at positions $R_1, \ldots, R_M$. The Schrödinger operator of such a system in appropriate units is

$$H(Z, R) \ = \ \sum_{i=1}^{N} \big(-\frac{1}{2}\Delta_i - V_Z(x_i, R) \big) + \sum_{i<j} |x_i - x_j|^{-1} \tag{1.1}$$

acting on $\bigwedge_{i=1}^{N} L^2({}^3 \times {}_2)$. Here $x_i \in {}^3$ is the coordinate of the i-th electron and Δ_i is the Laplacian in x_i, $Z = (Z_1, \ldots, Z_M)$, $R = (R_1, \ldots, R_M)$ and

$$V_Z(x, R) \ = \ \sum_{i=1}^{M} \frac{Z_i}{|x - R_i|} \ . \tag{1.2}$$

$V_Z(x, R)$ is potential of attraction of an electron to the nuclei situated at positions $R_1, \ldots, R_M$. Let

$$E(Z, R) \ = \ \inf \operatorname{spec} H(Z, R) \ ,$$

the ground state energy of $H(Z, R)$. In this paper we study an asymptotic behaviour of $E(Z, R)$ as $Z \to \infty$ along some direction in ^{M}.

L.H. Thomas and E. Fermi have suggested in 1927 that a large Coulomb system (atom or molecule) in the ground state ($=$ eigenfunction corresponding to the lowest eigenvalue) looks like a classical gas but with Pauli principle, namely, there could be at most 2 electrons per volume $(2\pi)^3$ in the phase space. Such an object is called now the *Thomas-Fermi gas.* Its states are described by the *electron density* $\rho \geq 0$ on ^{3} normalized as

$$\int \rho \ = \ N \ = \ \#\text{ of electrons.} \tag{1.3}$$

The energy of the Thomas-Fermi gas is given by a non-linear functional

$$\mathcal{E}^{\mathrm{TF}}(\rho) \;=\; \gamma \int \rho^{\frac{5}{3}} - \int V\rho + \frac{1}{2}\int \rho(|x|^{-1} * \rho) \;, \tag{1.4}$$

where $\gamma = \frac{3}{5}(3\pi^2)^{\frac{2}{3}}$ and $V(x,R)$ is given by (1.2). This functional is finite for $\rho \in L^{\frac{5}{3}} \cap L^1$ and is bounded from below on the set $S_N = \{\rho \in L^{\frac{5}{3}} \cap L^1 \mid \rho \geq 0 \text{ and } \int \rho = N\}$ (see a brief review of the Thomas-Fermi theory in section 2 and the classical works [LiebSim 1977 and Lieb 1981], which this review follows).

The ground state or Thomas-Fermi energy, $E^{\mathrm{TF}}(Z,R)$, is the infimum (in fact, minimum if $N \leq \Sigma Z_j$) of this functional on S_N. It has the following scaling property

$$E^{\mathrm{TF}}(Z,R) \;=\; \beta^{-7} E^{\mathrm{TF}}(\beta^3 Z, \beta^{-1} R) \;. \tag{1.5}$$

Let $|Z| = \Sigma Z_j$. Taking $\beta = |Z|^{-\frac{1}{3}}$ and using eqn (1.5), we obtain

$$E^{\mathrm{TF}}(Z,R) \;=\; |Z|^{\frac{7}{3}} E^{\mathrm{TF}}(\lambda, y) \;,$$

where $\lambda = |Z|^{-1} Z$ and $y = |Z|^{\frac{1}{3}} R$. This formula determines the dependence of $E^{\mathrm{TF}}(Z,R)$ on $|Z|$ in the case when λ and y are fixed. In the general case eqn (1.5) and [LiebSim 1977, thms V.3 and V.4] yield that

$$(\Sigma Z_j)^{\frac{7}{3}} E^{\mathrm{TF}}_{\mathrm{atom}}(1) \;\leq\; E^{\mathrm{TF}}(Z,R) \;\leq\; (\Sigma Z_j^{\frac{7}{3}}) E^{\mathrm{TF}}_{\mathrm{atom}}(1) \;, \tag{1.6}$$

where $E^{\mathrm{TF}}_{\mathrm{atom}}(\lambda)$ is the infimum of $\mathcal{E}^{\mathrm{TF}}(\rho)$ for $V(x) = \lambda |x|^{-1}$ on the set S_λ, i.e. the Thomas-Fermi energy of the "λ-atom". Note that $E^{\mathrm{TF}}_{\mathrm{atom}}(1)$ is independent of Z and R. If $Z \to \infty$ in a fixed direction and R obeys $\min_{i \neq j} |R_i - R_j| \geq |Z|^{-\nu}$ with $\nu < \frac{1}{3}$, then

$$E^{\mathrm{TF}}(Z,R) - \sum_{j=1}^{M} E^{\mathrm{TF}}_{\mathrm{atom}}(Z_j) \;=\; O(|Z|^{2+\nu}) \;, \tag{1.7}$$

This follows from (1.5) and [Lieb 1981, Thm 4.13].

The next theorem shows that the Thomas-Fermi theory is asymptotically correct for large Z systems but only to the leading order.

Theorem 1.1. *Let* $|Z| \to \infty$ *so that* $\min Z_j \geq \delta_1 |Z|$ *for* $\delta_1 > 0$ *independent of* Z *and let the mutual distances between* R_j *(which are allowed to depend on* Z *) be bounded from below by* $|Z|^{-\frac{5}{9}+\varepsilon}$ *with* $\varepsilon > 0$ *. Then for any* $\delta > 0$

$$E(Z,R) \;=\; E^{\mathrm{TF}}(Z,R) + \frac{1}{4}\sum Z_j^2 + O\big(a^{-\frac{1}{3}}|Z|^{\frac{16}{9}+\delta}\big)\ , \tag{1.8}$$

where $a = \min(|Z|^{\frac{1}{3}}|R_i - R_j|,\, i \neq j;\, 1)$ *and the estimate is uniform in the* $Z_j|Z|^{-1}$ *and in the* $|Z|^{\frac{1}{3}}R_j$ *.*

It will follow from the analysis below that the leading term on the r.h.s. represents the quasiclassical energy of the bulk of electrons and the second term, the quantum spectrum of Coulomb singularities.

The leading term in (1.6) was obtained in [LiebSim 1977] (see also Lieb 1981 and Thirr 1981). The second term of asymptotics was conjectured by J.M.C. Scott in 1952 as a contribution of those electrons which move very close to the nuclei (see [LiebSim 1977 and Lieb 1981] for a discussion). For atoms the Scott conjecture was proven in [Hughes 1990, SiedWeik 1987,1989] (see also [SiedWeik 1990]). Thus the new result of this paper is a proof of Scott conjecture for molecules. A proof of the next, $Z^{\frac{5}{3}}$ term for atoms is announced in [FeffSeco 1990]. The approach in [Hughes 1990, SiedWeik 1987,1989,1990, FeffSeco 1990] is based on an expansion in angular momentum channels. This is possible since the electron interaction with the nucleus $V(x,R)$, is spherically symmetric in atoms. The problem is then reduced to a one-dimensional one which is treated by the standard WKB method. The proof in this paper is rather general and is discussed below.

The philosophy of our approach is the same as that of Hughes-Siedentop-Weikard and can be discerned from [Lieb 1981]. Namely, on the first step the ground state energy of fully interacting electrons is approximated up to the order $O(|Z|^{\frac{5}{3}})$ by the ground state energy of independent Fermions moving in an effective exterior potential, $-\phi(x)$. The latter is composed of the original attractive potential between a given electron and the nuclei and an electro-static potential produced by an averaged out electron charge density.

This mean electron charge density must be found in a self-consistent way and it turns out to be the density which minimizes the Thomas-Fermi functional, i.e. the Thomas-Fermi density. We mention here that such an approach is rather common in Physics and is called the mean field approximation. After that the problem of finding the ground state energy of a system of N independent Fermions is reduced to determining the sum of the first N eigenvalues (counting the multiplicities, including those due to the spins) of the basic one-particle Schrödinger operator, $P = -\frac{1}{2}\Delta - \phi(x)$. A simple scaling maps the large $|Z|$ problem into the quasiclassical problem with $|Z|^{-\frac{1}{3}}$ playing the role of a Planck constant.

On the second step one studies quasiclassical asymptotics for the sum of the first N eigenvalues of P , or, in general, a class of one-particle Schrödinger operators whose potentials have Coulomb singularities. The point here is that the Weyl term of the asymptotics will be identified with the Thomas-Fermi contribution to the original ground state energy while the second term, with the Scott correction. The physics of the problem suggests that the second term should come from the singularities of the potential. The difficulty in finding such an asymptotic expansion is twofold. First of all the problem of determining the second term in the quasiclassical and spectral asymptotics is notoriously difficult (see e.g. [Hörm III, IV, Ivrii 1990-91, Robert 1987, Hux 1988, HelffRob 1990] and references therein). Secondly, all known approaches use pseudodifferential or Fourier integral operator Calculus and consequently require smooth potentials. Our method originates in general ideas of [Ivrii 1986, 1990-91], related to an approach of [Beals Feff 1974, Beals 1975] (see also [Tam 1984]).

There are two ingredients in our proof. First of all we estimate global quantities through local ones. For instance, we study

$$\operatorname{tr}\big(\psi(x)g(P)\big) \ , \tag{1.7}$$

where $g(\lambda) = \lambda$ for $\lambda \leq 0$ and $= 0$ for $\lambda \geq 0$. If $\psi \equiv 1$, then the trace above is just the sum of negative eigenvalues of P , the quantity we want to estimate. We take for ψ smooth functions localized outside of the singularities of the potentials. Then it is not difficult to obtain asymptotic expansion in the quasiclassical parameter β of the trace (1.7). Pseudodifferential calculus provides convenient tools for such a purpose. Adapting a standard technique, one represents $g(P)$ as

$$g(P) \;=\; \int \hat{g}(t) e^{-iPt} dt \;,$$

where $\hat{g}(t)$ is the Fourier transform of g. The evolution operator e^{-iPt} is then approximated for sufficiently small times and to any power in β by Fourier integral operators in the spirit of the geometrical optics. Such an approximation is possible because of finite speed of propagation of singularities (properly defined) for the Schrödinger equation, provided the energy is bounded from above (i.e. $\sup(\operatorname{supp} g) < \infty$) and the coordinate is localized in a domain in which the potential is bounded from below (cf. [SigSof 1988]). In the latter case, for sufficiently short times the bicharacteristics do not reach the singularities of ϕ. In fact, the Fourier integral operators in question are constructed to have C_0^∞ symbols and their analysis is well within the realm of the second year Calculus student. The approximating Fourier integral operators are then expanded by the method of stationary phase.

The second ingredient is a multiscale analysis. There are three scales in the problem: momentum scale determined by the quasiclassical parameter $\beta \sim |Z|^{-\frac{1}{3}}$, space scale, $\ell(x)$, determined by how the potential behaves under differentiation and the energy scale, $f(x)$, determined by the size of the potential. The first scale is constant while the other two depend on x. In our problem

$$\ell(x) \;=\; \text{dist. of } x \text{ to the singularities}$$

and $f(x) = \ell(x)^{-1}$. At each given point outside of the singularities we rescale the problem using the scales at this point in such a way that the problem is mapped into one on a unit ball with a smooth potential which is bounded together with all its derivatives independently of the scales involved and with a new quasiclassical parameter, α , defined in terms of the old one and all the scales. The new problem admits a quasiclassical expansion (in powers of α), as discussed above. This implies a quasiclassical expansion for the original problem outside of small balls around the singularities of the effective potential $\phi(x)$. The remainder in this expansion is bounded in terms of an explicit combination of all the scales times an absolute constant. The remarkable fact here is that since the subprincipal symbol of P is 0 , the second term in the asymptotic expansion is zero. In estimating the remainder the fact that the sum of the eigenvalues is given by the trace of a function of P which is once differentiable at the origin is crucial.

In a small ball around a singularity we replace our operator by one whose potential represents the leading singularity at this point. We estimate the spectral function of the new operator more carefully using its special form: that of hydrogen-type Hamiltonian. In fact, we use the spherical symmetry of the new potential. Similarly to the way [SiedWeik 1987,1989,1991] proceeded with the original problem we decompose our local trace into the angular momentum channels, use the explicit form of the eigenvalues to sum up the low angular momentum channels and our original quasiclassical expansion, in order to treat the high ones. At this stage, when we sum up explicitly the contribution of the low angular momentum channels of the Hydrogen Hamiltonian the Scott correction is produced.

Notation. We use the following standard conventions for the derivatives: $\partial_x = \mathrm{grad}_x$ (the gradient in x), $\partial_t = \frac{\partial}{\partial t}$, $\partial^2_{xt} = \partial_x \partial_t$, etc., and $\partial^\alpha_x = \prod\limits_{i=1}^{\dim} \partial^{\alpha_i}_{x_i}$ for a multi-index $\alpha = (\alpha_1, \alpha_2, \ldots)$. Moreover, ∇ will stand for the gradient in all the variables involved, $\| \cdot \|_1$ will denote the trace norm: $\|A\|_1 = \mathrm{tr}(A^* A)^{\frac{1}{2}}$ and $e_i(A)$ will stand for the i -th eigenvalue of a self-adjoint operator A , counting the multiplicities. $\langle x \rangle = (1 + |x|^2)^{\frac{1}{2}}$. In the rest of the paper C stands for various constants independent either of N , Z and R or of β and y , or of α .

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2. Mean Field Theory

In this section we reduce the problem of estimating the ground state energy of $H(Z,R)$ to one of finding the quasiclassical asymptotics for the sum of negative eigenvalues of an effective one-particle Hamiltonian. The latter describes the motion of a particle in the external Thomas-Fermi potential, i.e. the nuclear potential $V(x,R)$, screened by a mean electron charge distribution. In the rest of this section we use extensively results from the Thomas-Fermi theory of Coulomb systems. We refer the reader to [Lieb 1981] for an excellent review of the subject. Here we mention the following facts. In order to define the first term in $\mathcal{E}^{\mathrm{TF}}(\rho)$ one has to take $\rho \in L^{\frac{5}{3}}$. The physical origin of ρ dictates $\rho \in L^1$. This already suffices for $\mathcal{E}^{\mathrm{TF}}(\rho)$ to be well defined and bounded from below. To see this one observes that $|x|^{-1} \in L^{\frac{5}{2}} + L^{\infty}$ which implies that

$$\int |x|^{-1}\rho \;\leq\; C_1\|\rho\|_{\frac{5}{3}} + C_2\|\rho\|_1 \,.$$

The latter inequality yields that the second and the third terms in $\mathcal{E}^{\mathrm{TF}}(\rho)$ are finite in absolute value as well as that $\mathcal{E}^{\mathrm{TF}}(\rho)$ is bounded from below as

$$\begin{aligned}\mathcal{E}^{\mathrm{TF}}(\rho) \;\geq\; &\gamma\|\rho\|_{\frac{5}{3}}^{\frac{5}{3}} - C_1|Z|\|\rho\|_{\frac{5}{3}} \\ &- C_2|Z|\|\rho\|_1\end{aligned}$$

with C_1 and C_2 independent of Z, R and M. Furthermore, it is readily shown that $\mathcal{E}^{\mathrm{TF}}(\rho)$ defined on the set $L^1 \cap L^{\frac{5}{3}}$, $\rho \geq 0$ and $\int \rho = N$, is lower semicontinuous in the weak topology of $L^{\frac{5}{3}}$. This and Banach-Alaoglu theorem imply that the infimum of $\mathcal{E}^{\mathrm{TF}}(\rho)$ with the side conditions $\int \rho = |Z|$ and $\rho \geq 0$ is attained in $L^1 \cap L^{\frac{5}{3}}$. The inequality above shows that the L^p-norms with $1 \leq p \leq \frac{5}{3}$ of the ρ minimizing $\mathcal{E}^{\mathrm{TF}}(\rho)$ are bounded by $C|Z|^{\frac{9p-5}{4p}}$ with C independent of R and M.

Next, analyzing directly expression (1.4) for $\mathcal{E}^{\mathrm{TF}}(\rho)$, one sees that this functional is strictly convex

$$\mathcal{E}^{\mathrm{TF}}\big(t\rho_1 + (1-t)\rho_2\big) \;<\; t\mathcal{E}^{\mathrm{TF}}(\rho_1) + (1-t)\mathcal{E}^{\mathrm{TF}}(\rho_2)\;,$$

provided $0 < t < 1$ and $\rho_1 \neq \rho_2$. Since the set on which we minimize $\mathcal{E}^{\mathrm{TF}}(\rho)$ is also convex, we have that the minimizer of $\mathcal{E}^{\mathrm{TF}}(\rho)$ is unique.

According to Thomas and Fermi, for large N the electron density in the ground state is well approximated by some mean electron density, namely the one, $\rho_Z(x,R)$, which minimizes the Thomas-Fermi functional, $\mathcal{E}^{\mathrm{TF}}(\rho)$. Hence the potential experienced by any one electron is approximately

$$-\phi_Z(x,R) \;=\; -V_Z(x,R) + |x|^{-1} * \rho_Z \ , \tag{2.1}$$

i.e. one produced by the nuclei screened by this mean electron density. ϕ_Z is called the Thomas-Fermi potential; it will play an important role in our analysis. Using some convexity analysis one can show that the Euler-Lagrange equation for the minimizer ρ_Z is of the form

$$\rho_Z \;=\; \frac{2^{\frac{3}{2}}}{3\pi^2}\phi_Z^{\frac{3}{2}} \;>\; 0 \tag{2.2}$$

(provided $|Z| = N$) (see [LiebSim 1977, thms 11.20 and IV.3]). Note that the equation (2.1) implies that in the sense of distributions

$$-\Delta\phi_Z(x) \;=\; 4\pi\big(\Sigma Z_j\delta(x-R_j) - \rho_Z(x,R)\big) \ .$$

The Thomas-Fermi theory has a simple scaling property which we will use later. Using that

$$V_Z(x,R) \;=\; \beta^{-4}V_{\beta^3 Z}(\beta^{-1}x,\beta^{-1}R) \tag{2.3}$$

one concludes readily that the Thomas-Fermi functional for the potential $V_Z(x,R)$ evaluated at a density $\rho(x)$ equals β^{-7} times the Thomas-Fermi functional for the potential $V_{\beta^3 Z}(x,\beta^{-1}R)$ evaluated at the density $\beta^6\rho(\beta x)$. Using the uniqueness of the minimizer we conclude that

$$\rho_Z(x,R) \;=\; \beta^{-6}\rho_{\beta^3 Z}(\beta^{-1}x,\beta^{-1}R) \tag{2.4}$$

and that (1.5) holds. Using relation (2.4) together with either (2.1) and (2.3) or with (2.2), we conclude that

$$\phi_Z(x,R) \;=\; \beta^{-4}\phi_{\beta^3 Z}(\beta^{-1}x,\beta^{-1}R)\ . \tag{2.5}$$

The Thomas-Fermi energy $E^{\mathrm{TF}}(Z,R)$ is, in fact, the quasiclassical energy of a gas of $|Z|$ non-interacting Fermions in the external potential $-\phi_Z(x,R)$. Indeed, the quasiclassical Fermi energy of such a gas in the ground state is 0:

$$\begin{aligned} 2\int_{p\le 0} dx d\xi \;&=\; 2^{\frac{3}{2}}(3\pi^2)^{-1}\int \phi_Z(x,R)^{\frac{3}{2}}dx \\ &=\; \int \rho_Z(x,R)dx \;=\; |Z|\ , \end{aligned}$$

where $p(x,\xi) \;=\; \frac{1}{2}|\xi|^2 - \phi_Z(x,R)$, the classical Hamiltonian of a single Fermion. Here we have used Thomas-Fermi equation (2.2) and the normalization of ρ_Z. Hence the quasiclassical energy of this gas is

$$2\int_{p\le 0} p dx d\xi \;=\; -\frac{2}{15\pi^2}\int \phi_Z^{\frac{5}{3}}\ .$$

Now the Thomas-Fermi equation (2.3) implies

$$\int \phi_Z^{\frac{5}{3}} \;=\; (3\pi^2)^{\frac{5}{3}}\int p_Z^{\frac{5}{3}} \quad \text{and} \quad \int \phi_Z\rho_Z \;=\; (3\pi^2)^{\frac{2}{3}}\int \rho_Z^{\frac{5}{3}}\ .$$

The last three equations together with the definition of $E^{\mathrm{TF}}(Z,R)$ (see e.g. eqn (1.4)) yield

$$2\int_{p\le 0} p dx d\xi \;=\; E(Z,R) + D_{\mathrm{TF}}\ . \tag{2.6}$$

This relation is, in fact, the Virial theorem of the Thomas-Fermi theory (see [LiebSim 1977, thm II.23, Lieb 1981, thm 2.14]) and it is a consequence of a scaling property of the Thomas-Fermi potential under the map $\rho(x)\to t^3\rho(tx)$.

Our next task is to derive estimates on $\phi_Z(x,R)$ needed later. These estimates extend somewhat earlier results of [LiebSim 1977, thms IV.5, IV.10] and their proof proceeds along similar lines. To make future references more convenient we change the symbols for parameters and in the next theorem deal with $\phi_\lambda(x,y)$ instead of $\phi_Z(x,R)$. We introduce the scale functions

$$\ell(x) \equiv \ell(x,y) \equiv \min_j |x-y_j| , \tag{2.7}$$

$$f(x) = \ell(x)^{-\frac{1}{2}} \langle \ell(x) \rangle^{-\frac{3}{2}} . \tag{2.8}$$

Theorem 2.1. *The Thomas-Fermi potential* ϕ *is smooth (in* x *) outside the points* $y_1, \dots, y_M$ *and obeys the estimates*

$$|\partial^\nu \phi_\lambda(x,y)| \le C_\nu (\min \lambda_j)^{-|\nu|} f(x)^2 \ell(x)^{-|\nu|} \tag{2.9}$$

for any multi-index ν *and uniformly in* y *,* M *and in* λ *. Here* $\ell(x)$ *and* $f(x)$ *are defined in (2.7) and (2.8), respectively.*

Proof. We begin with

Lemma 2.2. *Denote by* $\phi_z^{at}(x)$ *the Thomas-Fermi potential of the* z *-atom. Then*

$$\begin{aligned} \sum \lambda_j \phi_{z=1}^{at}(x-y_j) &\le \phi_\lambda(x,y) \\ &\le \Big(\sum \lambda_j \phi_{z=1}^{at}(x-y_j)^{\frac{3}{2}} \Big)^{\frac{2}{3}} . \end{aligned} \tag{2.10}$$

Proof. We follow closely the proof of [LiebSim 1977, thm V.12]. We omit the subindex λ at ρ and ϕ. Note first that by the definition of $\phi_\lambda(x,y)$

$$\Delta\phi = 4\pi\Big(-\sum_{j=1}^{M} \lambda_j \delta(x-y_j) + \rho(x) \Big) .$$

Let $B = \{x \in {}^d \mid \rho(x) \ge \sum \lambda_j \rho_j(x)\}$, where $\rho_j(x) = \rho^{at}(x-y_j)$ with $\rho^{at}(x)$, the Thomas-Fermi density of the $(z=1)$-atom. Let $\psi = \phi - \sum \lambda_j \phi_j$, where $\phi_j = \phi_{z=1}^{at}(x-y_j)$. Then $-\Delta\psi = 4\pi(-\rho + \sum \lambda_j \rho_j)$ and therefore $-\Delta\psi < 0$ on B, i.e. ψ is subharmonic on B. Hence it attains its maximum either on ∂B or at infinity. Since $\psi = 0$ on ∂B and at ∞, we conclude that $\psi \le 0$ on B. On the other hand, $B \subseteq \{x \in {}^d \mid \psi(x) > 0\}$ and therefore $B = \phi$. The latter fact is equivalent to the inequality $\rho \le \sum \lambda_j \rho_j$, which, due to the Thomas-Fermi equation (2.2), can be written as the upper bound in (2.10).

To prove the lower bound in (2.10) we consider the same function ψ as above and the set $D = \{x \in {}^d \mid \psi(x) < 0\}$. Since $\sum \lambda_j \phi_j \le (\sum \lambda_j \phi_j^{\frac{3}{2}})^{\frac{2}{3}}$, which is true due to $\sum \lambda_j = 1$, we have that

$$\begin{aligned} \sum \lambda_j \rho_j - \rho \;&=\; \sum \lambda_j \phi_j^{\frac{3}{2}} - \phi^{\frac{3}{2}} \\ &\ge (\sum \lambda_j \phi_j)^{\frac{3}{2}} - \phi^{\frac{3}{2}} \; . \end{aligned}$$

Hence $\sum \lambda_j \rho_j - \rho > 0$ and therefore $-\Delta\psi > 0$ on D. Thus ψ is superharmonic on D. Consequently it takes its minimum on ∂D or at infinity. Since $\psi = 0$ on ∂D and at ∞, we have that $\psi \ge 0$ on D, i.e. $D = \phi$. Thus $\psi = \phi - \sum \lambda_j \phi_j \ge 0$, which is our lower bound.

Now the comparison argument, given in the proof of [LiebSim 1977, thm IV.10], applied to $\phi^{at}_{z=1}(x)$, yields

$$C_1 \min(|x|^{-1}, |x|^{-4}) \;\le\; \phi^{at}_{z=1}(x) \;\le\; C_2 \min(|x|^{-1}, |x|^{-4}) \tag{2.11}$$

for some (absolute) constants $0 < C_1 \le C_2 < \infty$. The latter inequality combined with (2.10) yields

$$C_1 (\min \lambda_j) f(x)^2 \;\le\; \phi_\lambda(x, y) \;\le\; C_2 f(x)^2 \; . \tag{2.12}$$

Hence by Thomas-Fermi equation (2.2), there are $0 < C_3 < C_4 < \infty$, independent of y and of λ, s.t.

$$C_3 (\min \lambda_j)^{\frac{3}{2}} f(x)^3 \;\le\; \rho_\lambda(x, y) \;\le\; C_4 f(x)^3 \; . \tag{2.13}$$

Now let $x_0 \notin \{y_j\}$, $\ell = (\min \lambda_j) \ell(x_0)$ and $f = f(x_0)$. In the rest of this proof $O(\ell^{-s})$, etc, stand for estimates uniform in β, y, λ and M. Let θ be smooth, supported in ${}^d \backslash B(x_0, \frac{2}{7}\ell)$ and $= 1$ in ${}^d \backslash B(x_0, \frac{1}{3}\ell)$ and obeying $\partial^\nu \theta = O(\ell^{-|\nu|})$. Then

$$V_\lambda - |x|^{-1} * (\theta \rho_\lambda) \;\equiv\; \phi_1$$

is a harmonic function in $B(x_0, \frac{1}{4}\ell)$. Writing it as a Poisson integral over the boundary of $B(x_0, \frac{1}{4}\ell)$, we obtain

$$\partial^\nu \phi_1 \;=\; O(f^2 \ell^{-|\nu|})$$

in $B(x_0, \frac{1}{5}\ell)$. On the other hand, by (2.13) and since $(1-\theta)\rho_\lambda$ is supported in $B(x_0, \frac{1}{3}\ell)$, we have

$$\partial^\nu \big(|x|^{-1} * (1-\theta)\rho_\lambda\big) \;=\; O(f^3 \ell^{2-|\nu|})$$

in $B(x_0, \frac{1}{5}\ell)$ for $|\nu| \le 1$. The last two relations yield

$$\partial^\nu \phi \;=\; O(f^2 \ell^{-|\nu|}) \tag{2.14}$$

in $B(x_0, \frac{1}{5}\ell)$ for $|\nu| \le 1$. By (2.2) we have that

$$\partial^\nu \rho_\lambda \;=\; O(f^3 \ell^{-|\nu|}) \tag{2.15}$$

for $|\nu| \le 1$. Using this and repeating the argument above we arrive at (2.14) for $|\nu| \le 2$. This together with (2.2) and (2.12) yields (2.15) for $|\nu| \le 2$. Iterating this procedure, we arrive at (2.14) and (2.15) in $B(x_0, \frac{1}{5}\ell)$ for all ν .

Equation (2.15) implies

$$|\partial^\nu \rho_\lambda(x,y)| \;\le\; C_\nu (\min \lambda_j)^{-|\nu|} f(x)^3 \ell(x)^{-|\nu|} \;, \tag{2.16}$$

which together with (2.1) yields (cf. [LiebSim 1977, thm IV.5])

$$\phi_\lambda(x,y) \;=\; \sum_j \frac{\lambda_j}{|x-y_j|} + \phi^{\mathrm{reg}}(x) \tag{2.17}$$

with $\phi^{\mathrm{reg}}(x)$ smooth outside $y_1, \ldots, y_M$ and obeying

$$|\partial^\nu \phi^{\mathrm{reg}}(x)| \;\le\; C_\nu (\min \lambda_j)^{-1-|\nu|} \ell(x)^{(\frac{1}{2}-|\nu|)_-} \langle \ell(x) \rangle^{-\frac{3}{2}+(\frac{1}{2}-|\nu|)_+} \;. \tag{2.18}$$

The Schrödinger operator of N independent Fermions moving in the effective external potential $-\phi_Z(x,R)$ is

$$H^{\mathrm{ind}}(Z,R) \;=\; \sum_{i=1}^{N} \big(-\frac{1}{2}\Delta_i - \phi_Z(x_i,R)\big) - D_{\mathrm{TF}} \tag{2.19}$$

acting on the Fermi space $\bigwedge_{i=1}^{N} L^2({}^3 \times {}_2)$. Here D_{TF} is the number compensating for overcounting the electron-electron interaction in ϕ_Z.

$$D_{\mathrm{TF}} \;=\; \frac{1}{2}\int\int \frac{\rho_Z(x,R)\rho_Z(y,R)}{|x-y|}dxdy \;. \tag{2.20}$$

Let $E^{\mathrm{ind}}(Z,R)$ be the ground state energy of $H^{\mathrm{ind}}(Z,R)$:

$$E^{\mathrm{ind}}(Z,R) \;=\; \inf\operatorname{spec} H^{\mathrm{ind}}(Z,R) \;.$$

The following theorem closely related to results of [Hughes 1990, NarnThirr 1981, SiedWeik 1987, 1989, FeffSeco 1990] obtained for atoms, is the main result of this section.

Theorem 2.3. *As* $|Z| \to \infty$ *so that* $\min Z_j \geq \delta|Z|$ *with* δ *independent of* Z, *the following relation holds uniformly in* R*:*

$$E(Z,R) \;=\; E^{\mathrm{ind}}(Z,R) + O\big(|Z|^{\frac{5}{3}}\big) \;. \tag{2.21}$$

Proof. We introduce the one-particle Schrödinger operator

$$P \;=\; -\frac{1}{2}\Delta - \phi_Z(x,R) \qquad \text{on} \;\; L^2({}^3 \times {}_2) \;. \tag{2.22}$$

Let $E_1, E_2, \ldots$ be the negative eigenvalues of P labelled counting their multiplicities in order of their increase and $\psi_1, \psi_2, \ldots$ be the corresponding eigenfunctions. We set $E_i = 0$ and $\psi_i = 0$ for $i >$ the total number of negative eigenvalues of P. Denote

$$\nu(x) \;=\; \sum_{i=1}^{N} |\psi_i(x)|^2 \tag{2.23}$$

and

$$\gamma(x,y) \;=\; \sum_{i=1}^{N} \psi_i(x)\overline{\psi_i(y)} \;. \tag{2.24}$$

Note that ν and γ are the one-particle density and one-particle density matrix, respectively for the ground state of $H^{\mathrm{ind}}(Z,R)$. In this section we use the shorthand

$$\int\int \frac{\rho(x)\sigma(y)}{|x-y|}dxdy \;\equiv\; \int\int \frac{\rho\sigma}{|x-y|} \;.$$

We begin with a result known to experts (see [Lieb 1979, NarnThirr 1981, SiedWeik 1987,1989]).

Theorem 2.4. *Let* $\mu = \nu - \rho_Z$. *Then there is a constant* C *independent of* Z *and* M *s.t.*

$$\begin{gathered}\frac{1}{2}\int\int\frac{\mu\mu}{|x-y|}-\frac{1}{2}\int\int\frac{|\gamma|^2}{|x-y|}\\ \geq E(Z,R)-E^{\mathrm{ind}}(Z,R)\geq -CM^{\frac{1}{2}}(\Sigma Z_j)^{\frac{5}{3}}\end{gathered}\tag{2.25}$$

Proof. We begin with a lower bound. Namely, we show that uniformly in Z , in M and in R

$$E(Z,R) \;\geq\; E^{\mathrm{ind}}(Z,R)-CM^{\frac{1}{2}}|Z|^{\frac{5}{3}} \;. \tag{2.26}$$

Let ψ be any function in $\bigwedge\limits_{i=1}^{N} L^2({}^3\times{}_2)$, normalized as $\sum\limits_{\text{spins}}\int|\psi|^2 \;=\; 1$. (Remember $N=|Z|$.) We associate with it the one-electron density

$$\rho_\psi(x_1) \;=\; N\sum_{\sigma_1,\ldots,\sigma_N}\int|\psi(x_1,\sigma_1\ldots,x_N,\sigma_N)|^2dx_2,\ldots,dx_N \;. \tag{2.27}$$

Note that

$$\int\rho_\psi \;=\; N \;.$$

It is shown in [Lieb 1979] that

$$\begin{gathered}\langle\psi,\sum_{i<j}|x_i-x_j|^{-1}\psi\rangle\\ \geq\frac{1}{2}\int\int\frac{\rho_\psi\rho_\psi}{|x-y|}-C\int\rho_\psi^{\frac{4}{3}}\end{gathered}\tag{2.28}$$

with C independent of N . To estimate the last term we use first the Hölder inequality

$$\begin{aligned}\int\rho_\psi^{\frac{4}{3}} \;&\leq\; (\int\rho_\psi^{\frac{5}{3}})^{\frac{1}{2}}(\int\rho_\psi)^{\frac{1}{2}}\\ &=\; N^{\frac{1}{2}}(\int\rho_\psi^{\frac{5}{3}})^{\frac{1}{2}}\end{aligned}\tag{2.29}$$

and then the Lieb-Thirring inequality (see e.g. [LiebThirr 1975])

$$\int\rho_\psi^{\frac{5}{3}} \;\leq\; \langle\psi,-\sum_{i=1}^{N}\Delta_i\psi\rangle \;. \tag{2.30}$$

Assume now that ψ is s.t.

$$\langle\psi,-\sum_{i=1}^{N}\Delta_i\psi\rangle \;\leq\; CMN^{\frac{7}{3}} \tag{2.31}$$

with the constant independent of N and M. Then

$$\int \rho_\psi^{\frac{4}{3}} \;\le\; C M^{\frac{1}{2}} N^{\frac{5}{3}} \; . \tag{2.32}$$

This together with (2.28) yields

$$\begin{aligned} &\langle \psi, \sum_{i<j} |x_i - x_j|^{-1} \psi \rangle \\ &\ge \frac{1}{2} \int\int \frac{\rho_\psi \rho_\psi}{|x-y|} - C M^{\frac{1}{2}} N^{\frac{5}{3}} \end{aligned} \tag{2.33}$$

with the constant independent of N and M. Now we transform

$$\begin{aligned} \frac{1}{2} \int\int \frac{\rho_\psi \rho_\psi}{|x-y|} \;&= \frac{1}{2} \int\int \frac{(\rho_\psi - \rho_Z)(\rho_\psi - \rho_Z)}{|x-y|} \\ &+ \int\int \frac{\rho_Z \rho_\psi}{|x-y|} - \frac{1}{2} \int\int \frac{\rho_Z \rho_Z}{|x-y|} \; , \end{aligned} \tag{2.34}$$

where, remember, ρ_Z is the Thomas-Fermi density. Combining the last two relations, we derive

$$\begin{aligned} &\langle \psi, \sum_{i<j} |x_i - x_j|^{-1} \psi \rangle \\ &\ge \int\int \frac{\rho_Z \rho_\psi}{|x-y|} - D_{\mathrm{TF}} \\ &+ \frac{1}{2} \int\int \frac{(\rho_\psi - \rho_Z)(\rho_\psi - \rho_Z)}{|x-y|} - C M^{\frac{1}{2}} N^{\frac{5}{3}} \; . \end{aligned} \tag{2.35}$$

Note that the first term on the r.h.s. can be written also as

$$\int\int \frac{\rho_Z \rho_\psi}{|x-y|} \;=\; \left\langle \psi, \left(\sum_{i=1}^{N} |x_i|^{-1} * \rho_Z \right) \psi \right\rangle \; . \tag{2.36}$$

The last two relations yield

$$\begin{aligned} &\langle \psi, H(Z,R) \psi \rangle \\ &\ge \langle \psi, \sum_{i=1}^{N} \big(-\frac{1}{2} \Delta_i - V_Z(x_i, R) + |x_i|^{-1} * \rho_Z \big) \psi \rangle \\ &- D_{\mathrm{TF}} + \frac{1}{2} \int\int \frac{(\rho_\psi - \rho_Z)(\rho_\psi - \rho_Z)}{|x-y|} - C M^{\frac{1}{2}} N^{\frac{5}{3}} \end{aligned} \tag{2.37}$$

with the constant independent of N and M.

Now we show (2.31) for any $\psi \in D(\sum \Delta_i)$ obeying $\langle \psi, H(Z,R)\psi\rangle \leq M|Z|^{\frac{7}{3}}$. We use that

$$M|Z|^{\frac{7}{3}} \;\geq\; \langle \psi, H(Z,R)\psi\rangle \;=\; \langle \psi, -\frac{1}{4}\sum_{i=1}^{N}\Delta_i\rangle + \langle \psi, H_1\psi\rangle \;, \tag{2.38}$$

where

$$H_1 \;=\; \sum_{i=1}^{N}\Big(-\frac{1}{4}\Delta_i - V_Z(x_i,R)\Big) + \sum_{i<j}|x_i - x_j|^{-1}$$

acting on $\bigwedge_{i=1}^{N} L^2(^2 \times {}_2)$. By the Lieb-Thirring bound ([LiebThirr 1975])

$$H_1 \;\geq\; -CM|Z|^{\frac{7}{3}} \tag{2.39}$$

with the constant independent of Z and M. Eqns (2.38) and (2.39) yield (2.31). Note that a bound, weaker than (2.39), namely with M replaced by M^2, is straightforward. Indeed

$$H_1 \;\geq\; T \;,$$

where

$$T \;=\; \sum_{i=1}^{N}\big(-\frac{1}{4}\Delta_i - V_Z(x_i,R)\big) \;, \tag{2.40}$$

acting on $\bigwedge_{i=1}^{N} L^2(^3 \times {}_2)$. This inequality is obtained by dropping from H_1 the positive electron-electron potential. Next, since (2.40) $= \sum_{j=1}^{M} A_j$, where $A_j = \sum_{i=1}^{N}\Big(-\frac{1}{2M}\Delta_i - \frac{Z_j}{|x_i - R_j|}\Big)$, the lowest eigenvalue of (2.40) is bounded from below by the lowest eigenvalue of

$$\sum_{i=1}^{N}\Big(-\frac{1}{2}\Delta_i - M|Z||x_i|^{-1}\Big)$$

acting on $\bigwedge_{i=1}^{N} L^2(^3 \times {}_2)$. The latter can be computed explicitly. It is 2 times the sum of the first $\frac{N}{2}$ eigenvalues (counting the multiplicities) of the operator $-\frac{1}{2}\Delta - M|Z||x|^{-1}$ on $L^2(^3)$ and is $O(M^2|Z|^{\frac{7}{3}})$. Then (2.37) holds for any $\psi \in D\big(\sum_{i=1}^{N} -\Delta_i\big)$ obeying $\langle \psi, H(Z,R)\psi\rangle \leq M|Z|^{\frac{7}{3}}$.

Using the definition of $H^{\rm ind}(Z,R)$ we rewrite eqn (2.37) as

$$\begin{aligned}\langle\psi, H(Z,R)\rangle \;&\geq\; \langle\psi, H^{\rm ind}(Z,R)\rangle\\ &+\frac{1}{2}\int\int\frac{(\rho_\psi-\rho_Z)(\rho_\psi-\rho_Z)}{|x-y|}-CM^{\frac{1}{2}}N^{\frac{5}{3}}\end{aligned}\tag{2.41}$$

and note that this equation implies (2.26).

Now we derive an upper bound on $E(Z,R)$. Let K be the minimum of N and the number of negative eigenvalues of P. Then, since $K\leq N$, we have by the HVZ theorem that

$$E(Z,R)\;\leq\; E_K(Z,R)\;,\tag{2.42}$$

where $E_K(Z,R)$ is the infimum of the spectrum of $H(Z,R)$ but with N replaced by K. On the other hand by the variational principle and our convention about the E_i 's and ψ_i 's.

$$E_K(Z,R)\;\leq\;\varepsilon^{\rm HF}(\Psi)\;,\tag{2.43}$$

where $\Psi=(\psi_1,\ldots,\psi_N)$ and $\varepsilon^{\rm HF}$ is the Hartree-Fock functional:

$$\begin{aligned}\varepsilon^{\rm HF}(\Psi)\;&=\;\sum_{i=1}^N\langle\psi_i,\big(-\frac{1}{2}\Delta-V_Z(\cdot,R)\big)\psi_i\rangle\\ &\quad+\frac{1}{2}\int\int\frac{\nu\nu}{|x-y|}-\frac{1}{2}\int\int\frac{|\gamma|^2}{|x-y|}\;,\end{aligned}\tag{2.44}$$

where ν and γ are defined in (2.23) and (2.24). We transform

$$\begin{aligned}\frac{1}{2}\int\int\frac{\nu\nu}{|x-y|}\;&=\frac{1}{2}\int\int\frac{\mu\mu}{|x-y|}\\ &\quad-\frac{1}{2}\int\int\frac{\rho_Z\rho_Z}{|x-y|}+\int\int\frac{\rho_Z\nu}{|x-y|}\;,\end{aligned}\tag{2.45}$$

where, recall, $\mu=\nu-\rho_Z$. Substituting this expression into (2.44), recalling definition (2.22) of P and remembering that ψ_i are the eigenfunctions of P corresponding to the eigenvalues E_i, we obtain

$$\begin{aligned}\varepsilon^{\rm HF}(\Psi)\;&=\;\sum_{i=1}^N E_i-D_{\rm TF}\\ &\quad+\frac{1}{2}\int\int\frac{\mu\mu}{|x-y|}-\frac{1}{2}\int\int\frac{|\gamma|^2}{|x-y|}\;.\end{aligned}\tag{2.46}$$

This together with (2.42) and (2.43) yields the upper bound from (2.7). Since the lower bound was proven in (2.26), this completes the proof of theorem 2.4.

Recall that we are interested in the asymptotic behaviour of $E(Z,R)$ as $Z \to \infty$ along a direction $\lambda = (\lambda_1, \ldots, \lambda_M)$, i.e. we set

$$Z_i \;=\; \lambda_i \beta^{-3} \;, \qquad i = 1, \ldots, M \tag{2.47}$$

with the λ_i 's fixed and β varying, $\beta \to 0$. Picking $\Sigma\lambda_i = 1$, we have $\beta = |Z|^{-\frac{1}{3}}$. Let $y = \beta^{-1} R$. Equation (2.5) can be rewritten as

$$\phi_Z(x,R) \;=\; \beta^{-4} \phi_\lambda(\beta^{-1}x, y) \;. \tag{2.48}$$

Now we rescale the operator P. Let

$$\big(U(\beta)\psi\big)(x) \;=\; \beta^{\frac{3}{2}} \psi(\beta x) \;, \tag{2.49}$$

the unitary family scaling $x \to \beta x$. Then for $Z = \beta^{-3}\lambda$ and $R = \beta y$

$$U(\beta) P U(\beta)^{-1} \;=\; \beta^{-4} K_\beta \;, \tag{2.50}$$

where K_β is the Schrödinger operator acting on $L^2({}^3 \times {}_2)$ and given by

$$K_\beta \;=\; -\frac{1}{2}\beta^2 \Delta_x - \phi_\lambda(x,y) \;. \tag{2.51}$$

Let $e_i(K)$ denote the i th eigenvalue of an operator K (counting the multiplicities) and let

$$k(x,\xi) \;=\; \frac{1}{2}|\xi|^2 - \phi_\lambda(x,y) \;. \tag{2.52}$$

For $\xi \in {}^d$, $d\xi$ will denote the Lebesgue measure divided by $(2\pi)^{-d}$.

Theorem 2.5. *Let K_β be defined in (2.51) with ϕ obeying (2.9). Let $\min \lambda_j \geq \delta$ with $\delta > 0$ independent of β. Then the number of eigenvalues of K_β not greater than $\mu \leq -\beta^A$ for some $A \geq 0$ verifies the following asymptotic expansion*

$$\#\{e_i(K_\beta) \leq \mu\} \;=\; 2\beta^{-3} \int_{k \leq \mu} dx d\xi + O(\beta^{-2}) \;. \tag{2.53}$$

Here the remainder estimate is uniform in μ, y *and in* λ.

Proof. The statement follows from theorem 8.9 with $s = 0$ and $d = 3$ from the relation

$$\#\{e_i(K_\beta) \leq \mu\} \;=\; \operatorname{tr} E(\mu, K_\beta) \tag{2.54}$$

where $E(\mu, A)$ is the spectral projection on $(-\infty, \mu]$ for an operator A. The factor 2 comes from the fact that K_β in theorems 2.4 and 8.6 acts on $L^2(^3 \times {}_2)$ and on $L^2(^3)$, respectively.

This result must be compared with analogous results in [Chaz 1980, Ivrii 1986, Rob 1987, Tam 1984] for assumptions on the potentials which are somewhat stronger than ours.

Remark 2.6. The leading terms in (2.53) can be computed more explicitly:

$$2 \int_{k \leq \mu} dx d\xi \;=\; \frac{2^{\frac{3}{2}}}{6\pi^2} \int (\phi_\lambda + \mu)_+^{\frac{3}{2}} dx \; . \tag{2.55}$$

Next, let $e_N = e_N(K_\beta)$ if $N \leq$ the total number of eigenvalues of K_β and $e_N = 0$ otherwise. In other words, e_N is the Fermi energy. Here $N = |Z| = \beta^{-3}$, the number of electrons.

Theorem 2.7. *(Estimate of the Fermi Energy) We have uniformly in the* y *and* λ

$$e_N \;=\; O(\beta^{\frac{4}{3}}) \; . \tag{2.56}$$

Proof. First, recall that ϕ_λ is the potential of the neutral Thomas-Fermi theory with $\sum \lambda_i$ electrons. Hence the Thomas-Fermi density ρ_λ satisfies (2.2) and

$$\int \rho_\lambda \;=\; \Sigma \lambda_i \; . \tag{2.57}$$

Now rewrite the expression (2.56) for $\mu = 0$:

$$\begin{aligned} 2 \int_{k \leq 0} dx d\xi \;&=\; \frac{2^{\frac{3}{2}}}{3\pi^2} \int \phi_\lambda^{\frac{3}{2}} dx \\ &=\; \Sigma \lambda_i \; . \end{aligned} \tag{2.58}$$

According to our convention e_N is either 0 or $e_N < 0$ and obeys, due to (2.58) and theorem 2.5 with $\mu = e_N$,

$$\beta^3 N \; = \; \frac{2^{\frac{3}{2}}}{3\pi^2} \int (\phi_\lambda + e_N)_+^{\frac{3}{2}} + O(\beta) \; . \tag{2.59}$$

Substracting (2.57) from this equation and remembering that $\beta^{-3}\Sigma\lambda_i = N$, we obtain

$$\int [(\phi_\lambda + e_N)_+^{\frac{3}{2}} - \phi_\lambda^{\frac{3}{2}}] \; = \; O(\beta) \; . \tag{2.60}$$

We estimate the l.h.s. from above. Remembering that $e_N \leq 0$, we obtain

$$\begin{aligned} &\int [\phi_\lambda^{\frac{3}{2}} - (\phi_\lambda + e_N)_+^{\frac{3}{2}}] \\ &\geq \int_{\phi_\lambda \leq -e_N} \phi_\lambda^{\frac{3}{2}} \; . \end{aligned} \tag{2.61}$$

This inequality together with eqns (2.12) and (2.60) shows already that $-e_N \leq 1$. Next, using (2.12), we derive

$$\int_{\phi_\lambda \leq -e_N} \phi_\lambda^{\frac{3}{2}} \; \geq \; \delta_1 (\min \lambda_j)^{\frac{3}{2}} \int_{\ell(x)^{-4} \leq -e_N} \ell(x)^{-6} \tag{2.62}$$

for some $\delta_1 > 0$ independent of β, of M, of the λ_j's and of the y_j's. Using an elementary estimate

$$\begin{aligned} &\int_{\ell(x) \geq \rho} \ell(x)^{-6} dx \; \geq \; \int_{2\rho \geq \ell(x) \geq \rho} \ell(x)^{-6} dx \\ &= \sum_j \int_{\substack{2\rho \geq |x - y_j| \geq \rho \\ \ell(x) = |x - y_j|}} |x - y_j|^{-6} dx \\ &\geq (2\rho)^{-6} \sum_j \mathrm{meas}\{x \mid \rho \leq \ell(x) \leq 2\rho, \; \ell(x) = |x - y_j|\} \\ &\geq (2\rho)^{-6} \mathrm{meas}\{x \mid \rho \leq \ell(x) \leq 2\rho\} \\ &= \frac{7\pi}{16} \rho^{-3} \; , \end{aligned}$$

we obtain furthermore

$$\int_{\phi_\lambda \leq -e_N} \phi_\lambda^{\frac{3}{2}} \; \geq \; \delta (\min \lambda_j)^{\frac{3}{2}} (-e_N)^{\frac{3}{4}} \tag{2.63}$$

with $\delta > 0$ independent of β, of M, of the λ_j 's and of the y_j 's. The last two inequalities imply

$$\int [\phi_\lambda^{\frac{3}{2}} - (\phi_\lambda + e_N)_+^{\frac{3}{2}}] \ \geq \ \delta (\min \lambda_j)^{\frac{3}{2}} (-e_N)^{\frac{3}{4}}$$

with δ independent of β and the y_j 's, which together with (2.60) implies (2.56).

Denote by $e(x, y, \mu, K_\beta)$ the Schwarz kernel of the spectral projection $E(\mu, K_\beta)$. Let

$$\begin{aligned} e_0(x, \mu, K_\beta) \ &= \beta^{-3} \int_{k \leq \mu} d\xi \ . \\ &= \beta^{-3} \frac{2^{\frac{3}{2}}}{3\pi^2} (\phi_\lambda + \mu)_+^{\frac{3}{2}} \ . \end{aligned} \tag{2.64}$$

We restate here corollary 11.7 from section 11 for $d = 3$.

Theorem 2.8. *Let K_β be the Schrödinger operator defined in (2.51) (and $d = 3$). Assume $\min \lambda_j \geq \delta$ with δ independent of β. Then for any $\mu \leq 0$*

$$\begin{aligned} &\Big(\int |e(x, x, \mu, K_\beta) - e_0(x, \mu, K_\beta)|^p dx \Big)^{\frac{1}{p}} \\ &\qquad \leq \ C \beta^{-2} \end{aligned} \tag{2.65}$$

with C independent of β, λ, y and μ.

We use this theorem in the proof of the following

Lemma 2.9. *Let, as above, $\mu = \nu - \rho_Z$, where ν is given in (2.5). Then*

$$\int \int \frac{\mu \mu}{|x - y|} \ \leq \ C |Z|^{\frac{5}{3}} \ . \tag{2.66}$$

Proof. Due to (2.51) we have for $Z = \beta^{-3} \lambda$ and $R = \beta y$

$$\psi_i(x) \ = \ \beta^{-\frac{3}{2}} \varphi_i(\beta^{-1} x) \ , \tag{2.67}$$

where φ_i are the eigenfunctions of K_β considered on $L^2(^3 \times {}_2)$ corresponding to the eigenvalues $e_i = e_i(K_\beta) = \beta^4 E_i$, if $i \leq$ the total number of eigenvalues of K_β, and $= 0$ otherwise. Hence

$$\sum_{i=1}^N |\psi_i(x)|^2 \ = \ \beta^{-3} \sum_{i=1}^N |\varphi_i(\beta^{-1} x)|^2 \ . \tag{2.68}$$

By the definition of e_N

$$\sum_{i=1}^{N} |\varphi_i(x)|^2 \ = \ e(x,x,e_N,K_\beta) \ , \tag{2.69}$$

where, recall, $e(x,y,\lambda,K_\beta)$ is the Schwartz kernel of $E(\lambda,K_\beta)$. Hence

$$\nu(x) \ \equiv \ \sum_{i=1}^{N} |\psi_i(x)|^2 \ = \ \beta^{-3} e(\beta^{-1}x,\beta^{-1}x,e_N,K_\beta) \ . \tag{2.70}$$

Next using (2.56) and (2.64) and the Thomas-Fermi equation (2.2), we find

$$e_0(x,e_N,K_\beta) \ = \ \beta^{-3}\rho_\lambda(x,y) + O\big(M^{\frac{4}{3}}\beta^{-\frac{5}{3}}|\phi|^{\frac{1}{2}}\big) \ . \tag{2.71}$$

Thus remembering the scaling property (2.48) of the Thomas-Fermi density and scaling relation (2.70), we derive

$$\mu(x) \ = \ \beta^{-3}\mu_1(\beta^{-1}x) \ , \tag{2.72}$$

where

$$\begin{aligned} \mu_1(x) \ &= e(x,x,e_N,K_\beta) \\ &\qquad - e_0(x,e_N,K_\beta) + O\big(\beta^{-\frac{5}{3}}\phi^{\frac{1}{2}}\big) \ . \end{aligned} \tag{2.73}$$

Using this, we rescale the integral

$$\int\int \frac{\mu\mu}{|x-y|} \ = \ \beta^{-1}\int\int \frac{\mu_1\mu_1}{|x-y|} \ . \tag{2.74}$$

Next, we apply the weak Young inequality

$$\int\int \frac{\mu_1\mu_1}{|x-y|} \ \leq \ C\|\mu_1\|_{6/5}^2 \ . \tag{2.75}$$

Next using (2.73), theorem 2.8 and the fact that $\int \phi^{\frac{3}{5}} < \infty$, we find

$$\|\mu_1\|_{\frac{6}{5}} \ \leq \ C\beta^{-2} \ . \tag{2.76}$$

Equations (2.74)–(2.76) imply (2.66).

Theorem 2.4 and lemma 2.9 yield equation (2.21). Theorem 2.3 is proven.

Remark 2.10. There is a trade-off between analysis of this section and that of section 8 required for theorem 2.5. The latter can be simplified (at the expense of the former) if one replaces the potential $\phi_\lambda(x,y)$ in definition (2.51) of K_β by a deformed potential $\phi_{\lambda,\beta}(x,y)$ which differs from $\phi_\lambda(x,y)$, more precisely, which changes the sign at large x. Such a potential can be defined as follows

$$\begin{aligned} \phi_{\lambda,\beta}(x,y) \; &= \phi_\lambda(x,y)\chi\big(\beta^{\frac{2}{3}}\ell_\beta(x,y)\big) \\ &\quad - \beta^2\ell_\beta(x,y)^{-1}\overline{\chi}\big(\beta^{\frac{2}{3}}\ell_\beta(x,y)\big) \ , \end{aligned} \tag{2.77}$$

where $\chi \in C_0^\infty()$ and is supported in $(-2,2)$ and $=1$ in $[0,1]$, $\overline{\chi} = 1-\chi$ and $\ell_\beta(x,y) = \omega_\beta(x) * \ell(x,R)$. Here $\omega_\beta(x) = \beta^{\frac{2}{3}}\varepsilon^{-1}\omega\Big(\frac{x}{\varepsilon\beta^{-\frac{2}{3}}}\Big)$ with $\varepsilon > 0$ sufficiently small and $\omega \in C_0^\infty$ and supported in $B(0,2)$ and $=1$ on $B(0,1)$. Equation (2.9) implies that the deformed potential $\phi_{\lambda,\beta}(x,y)$ obeys the estimates

$$|\partial^\nu\phi_{\lambda,\beta}(x,y)| \;\le\; C_\nu(\min\lambda_j)^{-|\nu|}f_1(x)^2\ell(x)^{-|\nu|} \ , \tag{2.78}$$

where

$$f_1(x) \;=\; \max\big(f(x),\beta\ell(x)^{-\frac{1}{2}}\big) \ . \tag{2.79}$$

3. TF Gas and Weyl Asymptotics

In this section we establish a quasiclassical asymptotics for the sum of negative eigenvalues of K_β as $\beta \to 0$. The proof is obtained by patching together results of sections 8–10. After that we relate the mentioned asymptotics for K_β to that for the ground state energy $E^{\text{ind}}(Z,R)$ as $Z \to \infty$. Combining this with theorem 2.1 we conclude that theorem 1.1 is valid.

Since $H^{\text{ind}}(Z,R)$ acts on $\bigwedge_{i=1}^{N} L^2({}^3 \times {}_2)$ and since the variables $x_1, \dots, x_N$ in it separate, we have

$$E^{\text{ind}}(Z,R) \;=\; \sum_{i=1}^{N} E_i - D_{\text{TF}} \;, \tag{3.1}$$

where, recall, E_i are the eigenvalues of P labelled in order of their increase and counting their multiplicity (see the paragraph after equation (2.22)). This is a well known relation in Quantum Physics and is a consequence of the Pauli principle: at most two electrons (the double degeneracy corresponding to ${}_2$) for an energy level. We begin with

Theorem 3.1. *Consider the Schrödinger operator K_β on $L^2({}^3)$ with a potential $\phi(x)$ obeying (2.7)–(2.9) with $a = \min\{|y_i - y_j|\,|i \neq j\} \geq \beta^{\frac{2}{3}-\varepsilon}$ for some $\varepsilon > 0$. Assume $\min \lambda_j \geq \delta_1$ with $\delta_1 > 0$ independent of β. Then for any $\delta > 0$*

$$\sum_{e_i \leq 0} e_i(K_\beta) \;=\; \text{Weyl} \;+\; \text{Scott} \;+\; O\big(a^{-\frac{1}{3}}\beta^{-\frac{4}{3}-\delta}\big) \;, \tag{3.2}$$

where the remainder estimate is uniform in the y_j 's and in λ_j 's, restricted as above

$$\text{Weyl} \;=\; \beta^{-3} \int\int_{k \leq 0} k \, dx d\xi \tag{3.3}$$

and

$$\text{Scott} \;=\; \frac{\Sigma\lambda_j}{8}\beta^{-2} \;. \tag{3.4}$$

Proof. Let

$$g(\sigma) \;=\; \begin{cases} \sigma & \text{if } \sigma \leq 0 \\ 0 & \text{if } \sigma > 0. \end{cases} \tag{3.5}$$

Then

$$\sum_{e_i \leq 0} e_i(K_\beta) \;=\; \operatorname{tr} g(K_\beta)\ . \tag{3.6}$$

Introduce a smooth partition of unity, $\psi_0, \ldots, \psi_M$,

$$\sum_{i=0}^{M} \psi_i \;=\; 1 \tag{3.7}$$

with the properties

$$\begin{aligned} &\text{for } i \geq 1,\ \ \psi_i \text{ is supported in } B(y_i, 2r) \\ &\psi_0 \ \text{ is supported in } {}^3\backslash \bigcup_{i=1}^{M} B(y_i, r)\ , \end{aligned} \tag{3.8}$$

where $r > 0$ obeys

$$\frac{1}{4}\beta^{1-\delta} \;\leq\; r \;\leq\; \frac{1}{3}a \tag{3.9}$$

for some $\delta > 0$. We will choose r later. Then

$$\operatorname{tr} g(K_\beta) \;=\; \sum_{i=0}^{M} \operatorname{tr}\big(\psi_i g(K_\beta)\big)\ . \tag{3.10}$$

Since g obeys the conditions of theorem 8.1 with $s = 1$, theorem 8.9 with $d = 3$ and $s = 1$ is applicable and yields

$$\begin{aligned} \operatorname{tr}\big(\psi_0 g(K_\beta)\big) \;&= \beta^{-3} \int\!\!\int g(k)\psi_0 dx d\xi \\ &\quad + O\big(\beta^{-1} r^{-\frac{1}{2}}\big)\ . \end{aligned} \tag{3.11}$$

By theorem 9.1 with $d = 3$

$$\begin{aligned} &|\operatorname{tr}\big(\psi_i g(K_\beta) - \psi_i g(K_{i,\beta})\big) \\ &- \beta^{-3} \int\!\!\int \psi\big(g(k) - g(k_i)\big) dx d\xi| \\ &\leq\; C(\beta^{-1} r^{-\frac{1}{2}} + a^{-1}\beta^{-2} r)\ , \end{aligned} \tag{3.12}$$

provided $\beta^{\frac{2}{3}-\delta} \leq r \leq \frac{1}{3}a$ for some $\delta > 0$, $i \geq 1$,

$$K_{i,\beta} \;=\; -\frac{1}{2}\beta^2 \Delta - \frac{\lambda_i}{|x - y_j|} \tag{3.13}$$

and

$$k_i(x,\xi) \;=\; \frac{1}{2}|\xi|^2 - \frac{\lambda_i}{|x-y_i|}\;. \tag{3.14}$$

Finally, by theorem 10.1

$$\begin{aligned} &\operatorname{tr}\psi_i g(K_{i,\beta}) \\ &= \beta^{-3}\int\!\!\int \psi_i g(k_i)\,dx d\xi \\ &-\frac{\lambda_j^2}{8}\beta^{-2} + O(\beta^{-1}r^{-\frac{1}{2}}) \end{aligned} \tag{3.15}$$

with $i \geq 1$.

Equations (3.12) and (3.15) yield for $i \geq 1$

$$\begin{aligned} |\operatorname{tr}\big(\psi_i g(K_\beta)\big) - \beta^{-3}\int\!\!\int \psi_i g(k)\,dx d\xi \\ + \frac{\lambda_i^2}{8}\beta^{-2}| \;\leq\; C(\beta^{-2}ra^{-1} + \beta^{-1}r^{-\frac{1}{2}})\;. \end{aligned} \tag{3.18}$$

This relation together with equations (3.10)–(3.11) implies

$$\begin{aligned} |\operatorname{tr} g(K_\beta) - \beta^{-3}\int\!\!\int g(k)\,dx d\xi \\ + \frac{1}{8}\Sigma\lambda_i^2\beta^{-2}| \;\leq\; C(\beta^{-2}ra^{-1} + \beta^{-1}r^{-\frac{1}{2}})\;. \end{aligned} \tag{3.19}$$

Comparing this with (3.6) and choosing $r = \beta^{\frac{2}{3}-\delta}a^{\frac{2}{3}}$, we arrive at (3.2).

Proof of theorem 1.1. First we show that

$$\#\{0 > e_i(K_\beta) > e_N\} \;=\; O\big(\beta^{-2}\big)\;. \tag{3.20}$$

Indeed, due to (2.53),

$$\begin{aligned} &\#\{0 > e_i(K_\beta) > e_N\} \\ &= \beta^{-3}\int_{0\geq k\geq e_N} dx d\xi + O\big(\beta^{-2}\big)\;. \end{aligned} \tag{3.21}$$

Equations (2.55) and (2.60) yield

$$\int_{0\geq k\geq e_N} dx d\xi \;=\; O\big(\beta\big)\;, \tag{3.22}$$

which together with (3.21) implies (3.20). Equations (3.20) and (2.53) yield

$$\begin{aligned}\sum_{i>N} |e_i(K_\beta)| \ &\leq \ |e_N| \#\{0 > e_i(K_\beta) > e_N\} \\ &\leq \ C\beta^{-\frac{2}{3}} \ .\end{aligned} \tag{3.23}$$

Recall that $k(x,\xi) \ = \ \frac{1}{2}|\xi|^2 - \phi_\lambda(x,y)$, where ϕ_λ is the potential of the neutral Thomas-Fermi theory with nuclei of charges $\lambda_1, \ldots, \lambda_M$ located at $y_1, \ldots, y_M$. Equations (2.5) and (2.6) yield

$$2\beta^{-3} \int\int_{k\leq 0} k dx d\xi \ = \ \beta^{-3} E^{\mathrm{TF}}(\lambda, y) + D_{\mathrm{TF}} \ . \tag{3.24}$$

Equations (3.23) and (3.24), together with (3.2), imply

$$\sum_{i=1}^{N} e_i(K_\beta) \ = \ \beta^{-3} E^{\mathrm{TF}}(\lambda, y) + \frac{\Sigma \lambda_i^2}{4} \beta^{-2} + D_{\mathrm{TF}} + O\big(a^{-\frac{1}{3}} \beta^{-\frac{4}{3}-\delta}\big) \ , \tag{3.25}$$

provided $|y_i - y_j| \geq \beta^{\frac{2}{3}-\varepsilon}$ for all $i \neq j$ and some $\varepsilon > 0$. Now, due to relation (2.50),

$$E_i \ = \ \beta^{-4} e_i(K_\beta) \ , \tag{3.26}$$

where E_i, recall, are the eigenvalues of P. Taking into account the scaling property of the Thomas-Fermi energy

$$E^{\mathrm{TF}}(Z, R) \ = \ \beta^{-7} E^{\mathrm{TF}}(\lambda, y) \ , \tag{3.27}$$

where $Z = \beta^{-3}\lambda$ and $R = \beta y$, we derive from (3.25) that

$$\sum_{i=1}^{N} E_i \ = \ E^{\mathrm{TF}}(Z, R) + \frac{\Sigma Z_i^2}{4} + D_{\mathrm{TF}} + O\big(a^{-\frac{1}{3}} |Z|^{\frac{16}{9}+\delta}\big) \ ,$$

provided $|R_i - R_j| \geq |Z|^{-\frac{5}{9}+\varepsilon}$ for all $i \neq j$ and some $\varepsilon > 0$. This relation together with equations (2.21) and (3.1) implies (1.8).

4. Energy Bounds

In this section we prove two kinds of estimates: bounds on the momentum in terms of energy and bounds on accessibility of energetically forbidden regions of the phase-space. Both bounds are needed in the following sections. Though the latter bounds have obvious classical meaning the operators involved are not pseudodifferential. In other words we obtain results, which normally follow from symbolic calculus, for non-symbolic operators. In a different context such results were obtained earlier in [SigSof 1987].

In this and the next three sections we consider a self-adjoint operator

$$H_\alpha \;=\; -\frac{\alpha^2}{2}\Delta - W(x)$$

on $L^2({}^d)$. Here $\alpha > 0$ is a quasiclassical parameter about which we assume only that $\alpha \le 1$. We assume that $W(x)$ is real, is in $L^2_{\rm loc}$ and obeys the Kato inequality

$$\|Wf\| \;\le\; \varepsilon\|\Delta f\| + \frac{C}{\varepsilon^2}\|f\| \tag{4.1}$$

for any $f \in D(\Delta)$ for any $\varepsilon > 0$ and with C independent of ε . (4.1) is satisfied for Kato potentials, i.e. the potentials from $L^p({}^d) + L^\infty({}^d)$ with $p > \frac{d}{2}$ for $d \ge 4$ and $p = 2$ for $d < 4$ (see e.g. [CFKS 1987]). Under the last restriction H_α is self-adjoint on $D(H_\alpha) = D(\Delta)$.

Note that a standard interpolation argument (see e.g. [RSII, thm IX.20] and (4.1) yield that

$$|\langle Wf, f\rangle| \;\le\; \varepsilon\langle -\Delta f, f\rangle + \frac{C}{\varepsilon^2}\|f\|^2 \tag{4.2}$$

(see e.g. [RSII, thm X.18]).

Lemma 4.1. *Let W obey (4.1). Then*

$$\|\Delta(H_\alpha + i)^{-1}\| \;\le\; C\max(\alpha^{-2}, \alpha^{-6}) \;, \tag{4.3}$$

$$\|\nabla(H_\alpha + i)^{-1}\| \;\le\; C\max(\alpha^{-1}, \alpha^{-2}) \tag{4.4}$$

and

$$\|\nabla(H_\alpha+i)^{-1}\nabla\| \;\le\; C\max(\alpha^{-2},\alpha^{-4}) \;. \tag{4.5}$$

Proof. Using

$$\|\Delta f\| \le \; 2\alpha^{-2}(\|H_\alpha f\|+\|Wf\|)$$

and (4.1) with $\varepsilon=\frac{1}{4}\alpha^2$, we obtain

$$\|\Delta f\| \;\le\; 4\alpha^{-2}\|H_\alpha f\|+C\alpha^{-6}\|f\|$$

which implies (4.3).

Next, let $u=(H_\alpha+i)^{-1}f$. Using that $\|\nabla u\|^2=\langle -\Delta u,u\rangle$, we obtain

$$\|\nabla u\|^2 \;=\; \frac{2}{\alpha^2}\big(\langle (H_\alpha+i)u,u\rangle+\langle (W-i)u,u\rangle\big) \;.$$

Applying (4.2) with $\varepsilon=\frac{\alpha^2}{4}$ to the last term, we obtain

$$\|\nabla u\|^2 \;\le\; \frac{2}{\alpha^2}|\langle (H+i)u,u\rangle|+\frac{1}{2}\|\nabla u\|^2+\frac{C}{\alpha^4}\|u\|^2 \;. \tag{4.6}$$

Since $(H+i)u=f$ and $\|u\|\le\|f\|$, this yields (4.4).

Finally, to prove (4.5) we note that (4.6) with $u=(H_\alpha+i)^{-1}\nabla f$ yields

$$\|\nabla u\|^2 \;\le\; \frac{4}{\alpha^2}\|f\|\|\nabla u\|+\frac{C}{\alpha^4}\|u\|^2 \;.$$

Since by the previous result $\|u\|\le C\alpha^{-2}\|f\|$, this yields (4.6).

In what follow $\|A\|_q=(\mathrm{tr}|A|^q)^{\frac{1}{q}}$, the I_q-trace norm of the operator A (see [RSII, p. 41] for the definition and properties used below).

Lemma 4.2. *Assume $W(x)$ obeys (4.1). Let $\psi\in C_0^\infty$ and $|\partial^\nu\psi(x)|\le C_\nu$. Let $n=\left[\frac{d}{2}\right]+1$. Then for $\alpha\le 1$*

$$\|\psi(H_\alpha+i)^{-n}\|_1 \;\le\; C\alpha^{-6n} \tag{4.7}$$

with C independent of α.

Proof. We conduct the proof by induction. As a result it is convenient to prove a more general statement:

$$\|\psi(H_\alpha + i)^{-m}\|_{\frac{n}{m}} \;\le\; C\alpha^{-6m} \;. \tag{4.8}$$

First we prove this statement for $m = 1$. By a property of the trace norms

$$\begin{aligned} &\|\psi(H_\alpha + i)^{-1}\|_n \\ &\le \|\psi(-\Delta + i)^{-1}\|_n \|(-\Delta + i)(H_\alpha + i)^{-1}\| \end{aligned} \tag{4.9}$$

Since $n > \frac{d}{2}$, then by a standard result the first factor on the r.h.s. is bounded. By (4.3), the second factor is bounded by $\mathrm{const} \cdot \alpha^{-6}$. Thus (4.8) with $m = 1$ follows.

Now we assume (4.8) is valid for some $m \ge 1$ and prove it for $m+1$. Let $\psi_1 \in C_0^\infty$, $= 1$ on $\operatorname{supp}\psi$, so that $\psi\psi_1 = \psi$, and obey $|\partial^\nu \psi_1(x)| \le C_\nu$. Using that

$$[\psi, (H_\alpha + i)^{-1}] \;=\; \alpha(H_\alpha + i)^{-1} L_\psi (H_\alpha + i)^{-1} \;, \tag{4.10}$$

where

$$L_\psi \;=\; -\alpha\nabla \cdot (\nabla\psi) - \frac{\alpha}{2}(\Delta\psi) \;, \tag{4.11}$$

and that $\psi = \psi_1\psi$, we obtain

$$\begin{aligned} \psi(H_\alpha + i)^{-m-1} \;&= \psi_1(H_\alpha + i)^{-1}\psi(H_\alpha + i)^{-m} \\ &\quad + \alpha\psi_1(H_\alpha + i)^{-1} L_\psi (H_\alpha + i)^{-m-1} \;. \end{aligned} \tag{4.12}$$

Writing $L_\psi = L_\psi\psi_1$ and repeating this procedure in the last term we arrive at

$$\begin{aligned} \psi(H_\alpha + i)^{-m-1} \;&= \psi_1(H_\alpha + i)^{-1}[\psi + \alpha L_\psi (H_\alpha + i)^{-1}\psi_1 \\ &\quad + \alpha^2 L_\psi (H_\alpha + i)^{-1} L_{\psi_1}]\psi_2(H_\alpha + i)^{-m} \;, \end{aligned} \tag{4.13}$$

where $\psi_2 = 1$ on $\operatorname{supp}\psi_1$ and obeys $\psi_2 \in C_0^\infty$, $|\partial^\nu\psi_2| \le C_\nu$. By lemma 4.1 the expression in the square brackets is bounded. Hence by a property of the trace norms

$$\begin{aligned} &\|\psi(H_\alpha + i)^{-m-1}\|_{\frac{n}{m+1}} \\ &\le C\|\psi_1(H_\alpha + i)^{-1}\|_n \|\psi_2(H_\alpha + i)^{-m}\|_{\frac{n}{m}} \;. \end{aligned} \tag{4.14}$$

By (4.8) with $m = 1$, proven above, and by the induction hypothesis the r.h.s. is bounded by $C\alpha^{-6(m+1)}$. This yields (4.8) with m replaced by $m+1$. The induction step is completed.

We will also need the following statement:

Lemma 4.3. *Assume W obeys (4.1). Let $\psi \in C^\infty$. Then*

$$\|\nabla\psi(H_\alpha + i)^{-1}\| \;\leq\; K\alpha^{-1} \;, \tag{4.16}$$

where $K = [(\sup_{\operatorname{supp}\psi} W)_+ + 1]^{\frac{1}{2}} \sup|\psi| + \alpha \sup|\nabla\psi|$.

Proof. Let $R = (H_\alpha + i)^{-1}$. We have

$$\begin{aligned} &\alpha^2 \frac{1}{2} R^*\psi^*\Delta\psi R \\ &\leq R^*\psi^* H_\alpha \psi R + \sup(W|\psi|^2) \;. \end{aligned} \tag{4.17}$$

Commuting H_α through ψ and using that

$$\begin{aligned} &\operatorname{Re}(R^*\psi^*[H_\alpha, \psi]R) \\ &= \alpha^2 R^*|\nabla\psi|^2 R \end{aligned}$$

and using that $\|H_\alpha R\| \leq 1$ we obtain that

$$\begin{aligned} &R^*\psi^* H_\alpha \psi R \\ &\leq \sup|\psi|^2 + \alpha^2 \sup|\nabla\psi|^2 \;. \end{aligned}$$

This together with (4.17) yields (4.16).

Next we have

Lemma 4.4. *Assume W obeys (4.1). Let ψ be smooth and obey $|\partial^\nu\psi(x)| \leq C_\nu$. Then*

$$\|\Delta\psi(H_\alpha + i)^{-1}\| \;\leq\; C\alpha^{-2}(\sup_{\operatorname{supp}\psi} |W| + 1) + 1 \;. \tag{4.18}$$

Proof. We have

$$\begin{aligned} &\|\Delta\psi(H_\alpha + i)^{-1} f\| \\ &\leq \frac{2}{\alpha^2}\|(H_\alpha + i)\psi(H_\alpha + i)^{-1} f\| \\ &\quad + \frac{2}{\alpha^2}(\sup_{\operatorname{supp}\psi} |W| + 1)\sup|\psi|^2 \|f\| \;. \end{aligned} \tag{4.19}$$

Commuting $(H_\alpha + i)$ through ψ, we obtain

$$\begin{aligned} &\|(H_\alpha + i)\psi(H_\alpha + i)^{-1} f\| \\ &\le \|\psi f\| + \alpha \|L_\psi (H_\alpha + i)^{-1} f\| \ . \end{aligned}$$

Applying lemma 4.3 to the last term we arrive at

$$\begin{aligned} &\|(H_\alpha + i)\psi(H_\alpha + i)^{-1} f\| \\ &\le C\big[\big(\alpha(\sup_{\operatorname{supp}\psi} W)_+ + 1\big)^{\frac{1}{2}} + \alpha^2 + 1\big]\|f\| \ . \end{aligned}$$

This together with (4.19) yields (4.18).

Proceeding as in the proof of lemma 4.2 but using lemmas 4.3 and 4.4 instead of lemma 4.1, one proves the following

Lemma 4.5. *Assume W obeys (4.1). Let $\psi \in C_0^\infty$ and obey $|\partial^\nu \psi| \le C_\nu$. Then for $n = \left[\frac{d}{2}\right] + 1$*

$$\|\psi(H_\alpha + i)^{-n}\|_1 \ \le \ C\alpha^{-2n}(\sup_\Omega |W| + 1)^n \ , \tag{4.20}$$

where Ω is $\varepsilon(\operatorname{diam}(\operatorname{supp}\psi))$ – neighbourhood of $\operatorname{supp}\psi$ and C independent of α.

Now we proceed to a less trivial result needed in this and forthcoming sections. This result shows how in the Operator Calculus we can pass from one Hamiltonian to another. Denote by $B(y,r)$ a ball in ^{d} of the radius r and centered at y.

Theorem 4.6. *Let (a) $H_\alpha = -\frac{\alpha^2}{2}\Delta - W(x)$ and $H_{0,\alpha} = -\frac{\alpha^2}{2}\Delta - W_0(x)$ with $W(x)$ and $W_0(x)$ obeying (4.1) and*

$$W(x) \ = \ W_0(x) \qquad \text{for } x \in B(0,2) \ , \tag{4.21}$$

(b) $\psi \in C_0^\infty(B(0,1))$ with $|\partial^\nu \psi(x)| \le C_\nu$ and (c) φ be smooth and obeying $|\partial^n \varphi(\lambda)| \le C_n \langle\lambda\rangle^{m-n}$. Then for any $A \ge \left[\frac{d}{2}\right] + 3$

$$\begin{aligned} &\|\psi(x)\big(\varphi(H_\alpha) - \varphi(H_{0,\alpha})\big)\|_1 \\ &\le C(\alpha L)^A \alpha^{-3d-12}\|\varphi\|_A \ , \end{aligned} \tag{4.22}$$

where $\|\varphi\|_A = \sup_\lambda(\langle\lambda\rangle^A|\partial_\lambda^{A+m}\varphi(\lambda)|)$, $L = \sup_{B(0,2)\backslash B(0,1)} \big(W(x)\big)_+^{\frac{1}{2}} + 1$ *and* C *is independent of* α *.*

Proof. We omit the subindex α in this proof: $H = H_\alpha$ and $H_0 = H_{0,\alpha}$. Let

$$\begin{aligned} U &= H - H_0 \\ &= W_0 - W \ . \end{aligned}$$

By (4.1) and (4.3)

$$\|U(H-z)^{-1}\| \ \leq \ C\alpha^{-6}\langle z\rangle|\mathrm{Im}\, z|^{-1} \ . \tag{4.23}$$

We begin with

Lemma 4.7. *Let* $\psi \in C_0^\infty(B(0,1))$ *and let* ψ_1 *be a smooth and bounded function supported in* ${}^d\backslash B(0,2)$ *. Then for any* $n \geq 0$ *and for any* $A \geq 0$

$$\|H^n\psi(H-z)^{-1}\psi_1\| \ \leq \ C(\alpha L|\mathrm{Im}\, z|^{-1})^A\langle z\rangle^n \tag{4.24}$$

and similarly for H_0 *. Here* C *is independent of* α *and* z *.*

Proof. Commuting H^n factor-by-factor through ψ and using that

$$[H,f] \ = \ \alpha L_f \ , \tag{4.25}$$

where L_f is defined in (4.11), we reduce the problem to one of showing that

$$\|\chi_1 H^m(H-z)^{-1}\psi_1\| \ \leq \ C(\alpha L|\mathrm{Im}\, z|^{-1})^A\langle z\rangle^m \tag{4.26}$$

for any $m \geq 0$ and any $A \geq 0$ and for C as above, provided $\chi_1 \in C_0^\infty\big(B(0,1+\varepsilon)\big)$ and $= 1$ on $B(0,1)$ and obeys $\partial^\nu\chi_1 = O(1)$ with $\varepsilon = \frac{1}{4A}$. Next, representing $H = H - z + z$ and using that $\chi_1\psi_1 = 0$, we reduce the problem further to showing that

$$\chi_1(H-z)^{-1}\psi_1 \ = \ O\big((\alpha L|\mathrm{Im}\, z|^{-1})^A\big) \ . \tag{4.27}$$

Now commuting χ_1 through $(H-z)^{-1}$ and using that $\chi_1\psi_1 = 0$, we obtain

$$\begin{aligned} &\chi_1(H-z)^{-1}\psi_1 \\ &= \alpha(H-z)^{-1}L_{\chi_1}\chi_2(H-z)^{-1}\psi_1 \end{aligned} \tag{4.28}$$

where $\chi_2 \in C_0^\infty\big(B(0,1+2\varepsilon)\big)$ and $=1$ on $B\big(0,1+\varepsilon\big)$ and χ_2 satisfies $\partial^\nu\chi_2 = O(1)$. Applying the above procedure to $\chi_2(H-z)^{-1}\psi_1$, etc., we arrive at

$$\chi(H-z)^{-1}\psi_1 \;=\; \alpha^A \prod_{i=1}^{A}[(H-z)^{-1}L_{\chi_i}](H-z)^{-1}\psi_1 \;, \tag{4.29}$$

where $\chi_k \in C_0^\infty\big(B(0,1+k\varepsilon)\big)$, $=1$ on $B\big(0,1+(k-1)\varepsilon\big)$ and obey $\partial^\nu\chi_k = O(1)$. Equation (4.16), the estimate $\partial^\nu\chi_i = O(1)$, the fact that $\nabla\chi_i$ are supported in $B(0,2)\backslash B(0,1)$ and the restriction $1 \geq \alpha^2$ imply that each factor on the r.h.s. is $O(|\mathrm{Im}\, z|^{-1}L)$. This yields (4.27). Hence (4.24) follows.

Now we proceed directly to the proof of theorem 4.6. There is a smooth function, ϕ, on ^{2}, supported in the strip $\{(\lambda,\mu)\;\big|\;|\mu|\leq 1\}$ and s.t. $\phi(\lambda,0)=\varphi(\lambda)$ and for any $A\geq 0$

$$|\partial_{\bar z}\phi(\lambda,\mu)| \;\leq\; \|\varphi\|_A|\mu|^{A+m-1}\langle\lambda\rangle^{-A} \;, \tag{4.30}$$

where $z=\lambda+i\mu$ and $\partial_{\bar z}=\partial_\lambda+i\partial_\mu$. To prove the existence of such a ϕ one uses a partition of unity associated with the length scale $\ell(\lambda)=\langle\lambda\rangle$ (see section 8) and then applies a standard extension theorem to each compactly supported piece of $\varphi(\lambda)$. Following [HSj 1989], one can represent

$$\varphi(A) \;=\; \frac{1}{2\pi i}\int\!\!\int \partial_{\bar z}\phi(A-z)^{-1}d\lambda d\mu \tag{4.31}$$

for any self-adjoint operator A. Using this representation, the second resolvent equation and the equation $H-H_0=U$, we find

$$\begin{aligned} &\varphi(H)-\varphi(H_0) \\ &= -\frac{1}{2\pi i}\int\!\!\int \partial_{\bar z}\phi\cdot(H-z)^{-1}U(H_0-z)^{-1}d\lambda d\mu \;. \end{aligned} \tag{4.32}$$

Denote $I_n=(H+i)^n\psi\big(\varphi(H)-\varphi(H_0)\big)$. Using this relation and the fact U is supported in ${}^d\backslash B(0,4)$, we transform

$$I_n \;=\; -\frac{1}{2\pi i}\int\!\!\int \partial_z\phi A(z)B(z)d\lambda d\mu \;, \tag{4.33}$$

where

$$A(z) \;=\; (H+i)^n \psi (H-z)^{-1} \psi_1 \;, \tag{4.34}$$

with ψ_1 , a smooth and bounded function supported in ${}^d \backslash B(0,3)$, and

$$B(z) \;=\; U(H-z)^{-1} \;. \tag{4.35}$$

By lemma 4.7, $A(z) = O\big((\alpha L |\mathrm{Im}\, z|^{-1})^M \langle z \rangle^n\big)$ for any M , and by (4.23), $B(z) = O(\alpha^{-2} \langle z \rangle |\mathrm{Im}\, z|^{-1})$. This together with (4.30) yields that

$$\|I_n\| \;\leq\; C \|f\|_M \alpha^{M-2} L^M \tag{4.36}$$

for any $M > n+1$.

Let now $\psi_2 \in C_0^\infty\big(B(0,2)\big)$ and $=1$ on $B(0,1)$. We write

$$\psi\big(\varphi(H) - \varphi(H_0)\big) \;=\; \psi_2 (H+i)^{-n} I_n \;. \tag{4.37}$$

Equations (4.20), (4.36) and (4.37) yield (4.22).

Denote $D_x = -i\alpha\, \mathrm{grad}_x$ and $D_t = i\alpha \frac{\partial}{\partial t}$. We assume now that in addition to (4.1), $W(x)$ is smooth in $B(0,2)$ and obeys

$$|\partial^\nu W(x)| \;\leq\; C_\nu \qquad \forall \nu \quad \text{on } B(0,2) \;. \tag{4.38}$$

We need the following microlocal estimate saying that operators are quasiclassically small in the classically forbidden region:

Theorem 4.8. *Assume W obeys (4.1) and (4.38). Let $g(\lambda)$ be a measurable function satisfying* $\sup(\mathrm{supp}\, g) < \infty$ *and* $|g(\lambda)| \leq C\langle \lambda \rangle^m$ *for some m and let $\varphi(x,\xi)$ be a smooth function supported in $B(0,1) \times {}^d$ and obeying $|\partial_x^\alpha \partial_\xi^\beta \varphi(x,\xi)| \leq C_{\alpha\beta} \langle \xi \rangle^{-|\beta|}$. Assume there is $\varepsilon > 0$ s.t.* $\mathrm{supp}\, \varphi \cap h^{-1}(\varepsilon\text{–}\mathrm{supp}\, g)$ *, where* $\varepsilon\text{–}Q = \{\lambda \in \;\big|\; \mathrm{dist}(\lambda, Q) \leq \varepsilon \langle \lambda \rangle\}$ *for $Q \subset$ and, recall, $h = \frac{1}{2}|\xi|^2 - W(x)$, the symbol of H_α . Then*

$$\|g(H_\alpha) \varphi(x, D_x)\|_1 \;=\; O(\alpha^A) \tag{4.39}$$

for any $A \geq 0$ *and any* $0 \leq \alpha \leq 1$.

Proof. Pick up $f(\lambda)$ smooth, supported in $\varepsilon - \operatorname{supp} g$ with ε given in the theorem and obeying $|\partial^n f(\lambda)| \leq C_n \langle\lambda\rangle^{m-n}$ and $f(\lambda) \geq |g(\lambda)|$. Using the definition of the trace norm (see e.g. [ReedSim II, p. 42]), we derive that

$$\|g(H_\alpha)\varphi(x, D_x)\|_1 \;\leq\; \|f(H_\alpha)\varphi(x, D_x)\|_1 \,.$$

Introduce an auxiliary potential $W_0(x)$ as

$$W_0 \in C_0^\infty(^d) \qquad \text{and} \qquad = W(x) \qquad \text{in } B\Big(0, \frac{3}{2}\Big)\,. \tag{4.40}$$

Let $\psi_1 \in C_0^\infty\big(B(0, 5/4)\big)$ and $= 1$ on $B(0, 6/5)$. Then by theorem 4.6

$$\|\big(f(H_\alpha) - f(H_{0,\alpha})\big)\psi_1(x)\|_1 \;\leq\; C\alpha^A$$

for any $A \geq 0$, where $H_{0,\alpha} = -\frac{\alpha^2}{2}\Delta - W_0(x)$. By the definition of α-pseudodifferential operators (see e.g. [Robert 1987])

$$\big(1 - \psi_1(x)\big)\varphi(x, D_x) \;=\; 0$$

for any $A \geq 0$. Next, due to the restrictons on f, since $H_{0,\alpha}$ is an elliptic α-pseudo-differential operator, then so is $f(H_{0,\alpha})$ (see [Robert 1987]). Moreover, the α-symbol of $f(H_{0,\alpha})$ is supported in $h^{-1}(\operatorname{supp} f)$. Hence using again α-pseudo-differential Calculus and trace norm estimates, we derive

$$\|f(H_{0,\alpha})\varphi(x, D_x)\|_1 \;\leq\; C\alpha^A$$

for any $A \geq 0$. The last four estimates yield (4.39).

Remark 4.9. We use theorem 4.8 in the following two situations:

a) $\varphi(x, \xi)$ is supported in $B(0, 1) \times \big(^d \backslash B(0, K)\big)$ and $g(\lambda)$ is smooth and supported in $|\lambda| \leq K_1$ with K_1 and K related as

$$K \;=\; (K_1 + 1)[(\sup_{B(0,2)} W)_+ + 2]^{\frac{1}{2}} \,.$$

b) $\varphi(x, \xi) = \psi(x)$ with $\psi(x) \in C_0^\infty\big(B(0, 1)\big)$ and $g(\lambda)$ is supported in $(-\infty, -\sup_{B(0,\rho)} W)$ for some $\rho > 1$.

Finally, we present the following rough estimate

Theorem 4.10. *Assume W obeys (4.1) and (4.38). Let g be a piecewise continuous function on obeying $|g(\lambda)| \leq C\langle\lambda\rangle^m$ for some m and $\sup(\operatorname{supp} g) < \infty$. Then for any $\psi \in C_0^\infty\big(B(0,1)\big)$*

$$\|\psi g(H_\alpha)\|_1 \ \leq \ C\alpha^{-d} \ . \tag{4.41}$$

Proof. Without a loss of generality one can assume g to be smooth. Let W_0 be a C_0^∞ potential satisfying (4.40). Introduce $H_{0,\alpha} = -\frac{1}{2}\alpha^2\Delta - W_0(x)$. Theorem 4.6 implies that

$$\|\psi\big(g(H_\alpha) - g(H_{0,\alpha})\big)\|_1 \ \leq \ C_A\alpha^A \tag{4.42}$$

for any $A \geq 0$. On the other hand, it is straightforward to show that for $n > \frac{d}{2}$

$$\|\psi(-\alpha^2\Delta + i)^{-n}\|_1 \ \leq \ C\alpha^{-d} \tag{4.43}$$

and then for any $n \geq 0$

$$\|(-\alpha^2\Delta + i)^n(H_{0,\alpha} + i)^{-n}\| \ \leq \ C \ . \tag{4.44}$$

The last two estimates yield

$$\|\psi g(H_{0,\alpha})\|_1 \ \leq \ C\alpha^{-d} \ . \tag{4.45}$$

Equations (4.42) and (4.45) yield (4.41).

5. Approximate Evolution

In this section and the next one we study behaviour of the evolution group

$$U(t) \; = \; e^{-iH_\alpha t/\alpha} \tag{5.1}$$

for small times. To this end we approximate $U(t)$, in the relevant part of the phase space, by a family of $F(t)$, of the Fourier integral operators in a spirit of geometrical optics and then estimate $F(t)$ by the stationary phase method (see [Lax 1957, Kell 1958, Masl 1965, Hörm 1968, Kum 1981, Chaz 1980]). In this section we construct $F(t)$ and study its properties. An important point here is that due to simple microlocal estimates of the previous section, $F(t)$ has a C_0^∞ symbol. This makes the investigation of $F(t)$ an exercise in Calculus.

We want to construct a Fourier integral operator

$$F(t)u \; = \; \alpha^{-d} \int\int e^{i\left(S(t,x,\xi)-z\cdot\xi\right)/\alpha} a(t,x,\xi,\alpha)u(z)dzd\xi \; , \tag{5.2}$$

satisfying (possibly, modulo terms supported outside $B(0,\frac{6}{5})$)

$$(D_t - H)F \; = \; O(\alpha^A)$$

for some $A > 0$ sufficiently large and

$$F(0) \; = \; \varphi(x, D_x) \; , \tag{5.3}$$

where $\varphi \in C_0^\infty\left(B(0,\frac{5}{4}) \times B(0,K)\right)$, with a fixed K chosen later, and is even in ξ. Note that after taking the Fourier integral in z, the remaining ξ-integral in (5.2) is absolutely convergent (for sufficiently small times, see the paragraph before eqn (5.10)). Let

$$h(x,\xi) \; = \; \frac{1}{2}|\xi|^2 - W(x) \; .$$

Clearly, estimating $(D_t - H)F(t)$ reduces to evaluating $(D_t - H)(ae^{\frac{iS}{\alpha}})$. Taking S independent of α and equating the coefficient at α^0 in this expression to 0 leads to

$$\partial_t S + h(x, \partial_x S) \; = \; 0 \; , \tag{5.4}$$

the Hamilton-Jacobi equation. The initial condition is

$$S|_{t=0} \; = \; x \cdot \xi \; . \tag{5.5}$$

Next, picking a of the form

$$a \; = \; \sum_{j=0}^{N} \alpha^j a_j(t,x,\xi) \tag{5.6}$$

with $N = M-1$ and equating the coefficients in $(D_t - H)(ae^{\frac{iS}{\alpha}})$ at α^j , $j = 1,\ldots,N+1$, to zero leads to the transport equations

$$\partial_t a_j + \partial_x S \cdot \partial_x a_j + \frac{1}{2}\Delta_x S a_j \; = \; -\frac{i}{2}\Delta_x a_{j-1} \tag{5.7}$$

for $j \geq 0$ and with $a_{-1} = 0$ and with the initial conditions

$$a_j|_{t=0} \; = \; \delta_{j,0}\varphi \; . \tag{5.8}$$

The initial conditions yield

$$ae^{iS/\alpha}|_{t=0} \; = \; \varphi e^{ix\cdot\xi/\alpha} \; , \tag{5.9}$$

which guarantees, due to the relation

$$\alpha^{-d} \int\int e^{i(x-z)\cdot\xi/\alpha}\varphi(x,\xi)u(z)dzd\xi \; = \; \varphi(x,D_x)u(x) \; ,$$

that $F(0) = \varphi(x, D_x)$.

The Hamilton-Jacobi equations (5.4)–(5.5) and the transport equations (5.7)–(5.8) can be solved by the method of characteristics (see e.g. [Arn 1989, Chaz 1980, Kum 1981]). For instance, the unique solution of the Hamilton-Jacobi equations is given for $|t|$ sufficiently small by the action function

$$S(t,x,\eta) \; = \; z \cdot \eta + \int (\xi \cdot dx - h)$$

along the classical trajectory for the Hamiltonian $h(x,\xi)$ with the momentum η at time $s = 0$ and the position x at time $s = t$. Here z is the position at time $s = 0$ as a function of t, x and η. Fix the degree of approximation N. Let $T_1 > 0$ (depending of K) be such that the Hamiltonian flow for $h(x,\xi)$ starting in $B(0,\frac{3}{2}) \times B(0,K+2)$ (resp. $B(0,\frac{5}{4}) \times B(0,K)$) exists for $|t| \leq T_1$ and stays during this period inside of $B(0,2) \times {}^{d}$ (resp. $B(0,\frac{4}{3}) \times B(0,K+1)$). Then decreasing T_1 depending on N, if necessary, we conclude that (5.4)–(5.5) and (5.7)–(5.8) with $j \leq N$ have unique solutions in $B(0,\frac{3}{2})$ for $\xi \in B(0,K+2)$ and $a_j \in C_0^\infty\big(B(0,\frac{4}{3}) \times B(0,K+1)\big)$ for $|t| \leq T_1$. Hence $a \in C_0^\infty\big(B(0,\frac{4}{3}) \times B(0,K+1)\big)$ for $|t| \leq T_1$. Thus $F(t)$ is well defined and obeys (5.3).

The expression $(D_t - H)F(t)$ will be estimated in the next section. In this section we study the asymptotic behaviour of $F(t)$. In what follows we assume that $T \leq T_1$. Let $\hat{\chi} \in C_0^\infty([-T,T])$. Then the operator

$$F_\chi(\lambda) \;=\; \int F(t)\hat{\chi}(t)e^{i\lambda t/\alpha}dt \tag{5.10}$$

is well-defined and, due to the fact that $a \in C_0^\infty$, is trace class.

Theorem 5.1. *If $\lambda < -\sup_{B(0,2)} W - 1$, then for any $A \geq 0$ and uniformly in λ*

$$\|F_\chi(\lambda)\|_1 \;=\; O(\alpha^A)\ . \tag{5.11}$$

Let η be smooth and bounded on ^{d} and supported in $|\xi| \geq K_0$, where $K_0 \geq 2(\sup_{B(0,2)} W + \lambda + 1)_+^{\frac{1}{2}}$, and let $T \leq \min(\delta K_0^{\frac{1}{2}}, T_1)$ with δ sufficiently small and independent of K_0 and K. Then for all λ

$$\|F_\chi(\lambda)\eta(D_x)\|_1 \;=\; O(\alpha^A) \tag{5.12}$$

for any $A \geq 0$.

Proof. The integral kernel of $F_\chi(\lambda)\eta(D_x)$ is

$$\int\!\!\int \hat{\chi} a \eta e^{i\phi_1/\alpha} d\xi\, dt$$

where $\phi_1 = S - z\cdot\xi + \lambda t$ and the remaining abbreviation is obvious. The Hamilton-Jacobi equation for S, the relation $\partial_x S = \xi + O(t)$ and the condition $T \leq \delta K_0^{\frac{1}{2}}$ imply

$$-\partial_t S \;\geq\; \frac{1}{4}K_0^2 - \sup_{B(0,2)} W$$

and therefore $-\partial_t\phi_1 \geq 1$ on $\operatorname{supp}(\hat{\chi}a\eta)$. Integrating by parts using the relation

$$Le^{i\phi_1/\alpha} \;=\; e^{i\phi_1/\alpha} \;,$$

where

$$L \;=\; -(\partial_t S + \lambda)^{-1} D_t \;,$$

we obtain (5.12). Equation (5.11) is proven similarly if one observes that

$$-\partial_t\phi_1 \;\geq\; -\lambda - \sup_{B(0,2)} W$$

on $\operatorname{supp} a$.

Let $\chi \in C_0^\infty([-T,T])$ and $\psi \in C^\infty(^d)$ and consider the function

$$I(\lambda,\alpha) \;=\; \operatorname{tr}\psi \int F(t)\hat{\chi}(t)e^{i\lambda t/\alpha}dt \;. \tag{5.13}$$

Due to theorem 5.1, for any $A \geq 0$

$$I(\lambda,\alpha) \;=\; O\Big(\big(\frac{\alpha}{|\lambda|}\big)^A\Big) \qquad \text{if} \quad \lambda < -\sup_{B(0,1)} W - 1 \;. \tag{5.14}$$

Using the Fourier integral representation of $F(t)$, we rewrite $I(\lambda,\alpha)$ as

$$I(\lambda,\alpha) \;=\; \alpha^{-d}\int\int\int e^{i\phi/\alpha}b\,dtdxd\xi \;, \tag{5.15}$$

where

$$b \;=\; \psi\hat{\chi}a$$

and

$$\phi(t,x,\xi) \;=\; S(t,x,\xi) - x\cdot\xi + \lambda t \;. \tag{5.16}$$

In the rest of this section y stands for a phase-space point $(x,\xi) \in {}^{2d}$ and $dy = dxd\xi$.

Let $\mathcal{E}_\lambda = \{y|h(y) = \lambda\}$, the energy shell at the energy λ. If $\nabla h \neq 0$ on $\mathcal{E}_\lambda \cap \operatorname{supp}\varphi$, then there is $\tau > 0$ (depending, in general, on the restriction of $|\nabla h|^{-1}$ to $\mathcal{E}_\lambda \cap \operatorname{supp}\varphi$) s.t. no periodic orbit of h with a period in $(0,\tau]$ passes through points of $\operatorname{supp} a$. This well-known statement follows from the beginning of the proof of theorem 5.2 below (see the paragraph containing eqn (5.23)). The next result is rather standard, we give its proof for the sake of completeness.

Theorem 5.2. *Let $\hat\chi$ be a smooth function, supported in $[-\tau,\tau]$ and obeying $\hat\chi(0)=1$ and $\hat\chi^{(k)}(0)=0$ for $k=1,2$ and let $\varphi\in C_0^\infty\big(B(0,\frac54)\times B(0,K)\big)$. Let λ be a regular value of h on $\operatorname{supp} a$. Then*

$$I(\lambda,\alpha) \;=\; 2\pi\alpha^{1-d}\int_{\mathcal{E}_\lambda}\psi\varphi dS_\lambda + O(\alpha^{3-d})\ , \tag{5.17}$$

where dS_λ is the h-induced area element of the surface $\mathcal{E}_\lambda$, i.e. $dS_\lambda=|\nabla h|^{-1}\times$ (Riemannian surface measure on $\mathcal{E}_\lambda$).

Proof. In order to prove (5.17) we use the method of stationary phase. We begin with a study of the critical manifold of ϕ. First, we claim that if $\nabla h\neq 0$ on $\mathcal{E}_\lambda\cap\operatorname{supp} a$ and if t is sufficiently small, then the critical manifold of ϕ is

$$C_\lambda \;=\; \{0\}\times\mathcal{E}_\lambda\ . \tag{5.18}$$

Indeed, since

$$\phi|_{t=0} \;=\; 0\ , \tag{5.19}$$

we have that

$$\partial_y\phi|_{t=0} \;=\; 0\ . \tag{5.20}$$

Next, by the Hamilton-Jacobi equation

$$\begin{aligned}\partial_t\phi \;&=\; \partial_t S+\lambda\\ &=\; -h(x,\partial_x S)+\lambda\ .\end{aligned}$$

This and the initial condition $S|_{t=0}=x\cdot\xi$ yield

$$\partial_t\phi|_{t=0} \;=\; -h+\lambda\ . \tag{5.21}$$

Hence

$$\partial_t\phi \;=\; 0 \quad \text{on} \quad C_\lambda\ .$$

Using (5.21), the fact that ϕ is smooth in all its variables on $\operatorname{supp} a$ and that $\operatorname{supp} a$ is compact, we obtain

$$\partial_t\phi \;=\; -h+\lambda+O(t)$$

on $\operatorname{supp} a$. Here and below $O(t^n)$ stands for a smooth symbol of the order $|t|^n$ on $\operatorname{supp} a$. Moreover, (5.21) yields

$$\partial^2_{yt}\phi\,\big|_{t=0} = -\nabla h \ , \tag{5.22}$$

which together with (5.20) implies that

$$\partial_y \phi \;=\; -\nabla h t + O(t^2)$$

on $\operatorname{supp} a$. Hence if $|t|$ is sufficiently small, then (5.18) exhausts all the critical points of ϕ on $\operatorname{supp} a$.

To see how large $|t|$ can be taken, we study the critical points of ϕ more carefully. Due to (5.16), the critical points (t, x, ξ) of ϕ obey the equations

$$\begin{aligned} \partial_t S \;&=\; -\lambda \\ \partial_x S \;&=\; \xi \\ \partial_\xi S \;&=\; x \ . \end{aligned} \tag{5.23}$$

Since S satisfies the Hamilton-Jacobi equation with the Hamiltonian function h and the initial condition $S|_{t=0} = x \cdot \xi$, we have that

$$\nabla_{(x,\xi)} S(t,x,\xi) \;=\; (\eta, z) \ , \quad \text{provided } \phi_t(z,\xi) \;=\; (x,\eta) \ ,$$

where ϕ_t is the flow generated by the Hamiltonian function h. Hence if (t_0, y_0) is a solution of (5.23), then t_0 is a period of a periodic orbit of ϕ_t passing through y_0 with the energy

$$h(y_0) \;=\; -(\partial_t S)(t_0, y_0) \;=\; \lambda \ .$$

Thus, we have shown that (i) the critical manifold of ϕ is the union of C_λ and the set of all points (t, y) s.t. $t \neq 0$, $y \in \mathcal{E}_\lambda$ and there is a periodic orbit through y which has the period t and (ii) if λ is not a critical value of h on $\operatorname{supp} a$, then there is an interval I around $t = 0$ (depending on $\operatorname{supp} a$) s.t. the critical manifold of ϕ on $I \times \operatorname{supp} a$ is $C_\lambda \cap (I \times \operatorname{supp} a)$. In particular, this implies that under the above condition on h and

λ there are no periodic orbits of ϕ_t through $\operatorname{supp} a$ with sufficiently small periods and therefore τ defined in the paragraph before theorem 5.2 is positive and C_λ is the critical manifold of ϕ on $\operatorname{supp} \hat{\chi} \times \operatorname{supp} a$.

Next, we compute the Hessian, ϕ'', of ϕ on the critical manifold (5.18). First, we note that

$$\partial_t^2 \phi|_{t=0} \;=\; -\xi \partial_x W \; . \tag{5.24}$$

Indeed, using twice that S is a solution to the Hamilton-Jacobi equation, we obtain

$$\begin{aligned}
\partial_t^2 S &= -\partial_t \left(\frac{1}{2} (\partial_x S)^2 - W(x) \right) \\
&= -\partial_x S \partial_{xt}^2 S \\
&= \partial_x S \partial_x \left(\frac{1}{2} (\partial_x S)^2 - W(x) \right) \\
&= \partial_x S (\mathrm{Hessian}_x S) \partial_x S - \partial_x S \partial_x W \; .
\end{aligned}$$

Applying now the initial condition $S|_{t=0} = x \cdot \xi$ and remembering that $\partial_t^2 \phi = \partial_t^2 S$, we arrive at (5.24).

Next, since $\phi|_{t=0} = 0$, we get that

$$\partial_{yy}^2 \phi|_{t=0} \;=\; 0 \; .$$

This relation together with (5.22) and (5.24) yield

$$\phi''|_{t=0} \;=\; - \begin{pmatrix} \xi \cdot \nabla W & \nabla h \\ (\nabla h)^T & 0 \end{pmatrix} \; , \tag{5.25}$$

where ∇h and $(\nabla h)^T$ stand for row and column vectors, respectively, and 0, for the $2d \times 2d$ zero matrix. A simple computation shows that $\phi''(\sigma)$ with $\sigma \in C_\lambda$ is non-degenerate on $N_\sigma \equiv T_\sigma{}^d \ominus T_\sigma C_\lambda$. Finally, the determinant of the restriction of $\phi''|_{t=0}$ to N_σ is

$$\det{}_N(\phi|_{t=0}) \;=\; -|\nabla h|^2 \tag{5.26}$$

and the signature of this restriction, which is the difference between the number of positive and negative eigenvalues, is

$$\mathrm{sign}_N(\phi''|_{t=0}) \;=\; 0 \; .$$

Since the restriction of $\phi''(\sigma)$, $\sigma \in C_\lambda$, to N_σ is non-degenerate, a stationary phase theorem is applicable to the integral (5.15) and it produces (see Appendix)

$$\begin{aligned} I(\lambda,\alpha) \;&=\; 2\pi\alpha^{1-d}\sum_{k=0}^{N-1} k!^{-1}\int_{\mathcal{E}_\lambda}\left[|\nabla h|^{-1}\left(\frac{i}{2}\alpha L\right)^k (b\rho e^{i\theta/\alpha})\right]_{C_\lambda} dS_\lambda \\ &\quad + O(\alpha^{N+1-d}) \;, \end{aligned} \tag{5.27}$$

where, with $\phi''(\sigma)^{-1}$ standing for the inverse of the restriction of $\phi''(\sigma)$ to N_σ , $\sigma \in C_\lambda$,

$$L \;=\; \langle \phi''(\sigma)^{-1}\nabla, \nabla\rangle \;, \tag{5.28}$$

with ∇ , the gradient in t and y , ρ is a smooth function of x and $|\xi|$ obeying

$$\rho \;=\; |\nabla h| \qquad \text{on} \qquad \mathcal{E}_\lambda \;, \tag{5.29}$$

dS_λ is the h-induced surface measure on $\mathcal{E}_\lambda$ ($= |\nabla h|^{-1}\times$ the natural surface measure on $\mathcal{E}_\lambda$),

$$\theta \;=\; \phi(z) - \phi(\sigma) - \frac{1}{2}\langle z-\sigma, \phi''(\sigma)(z-\sigma)\rangle \tag{5.30}$$

with $z=(t,y)\in N_\sigma$ and $\sigma \in C_\lambda$. Here we have identified C_λ with $\mathcal{E}_\lambda$.

We will use the expansion above for $N=2$ and we compute explicitly its first two terms. Since

$$b|_{t=0} \;=\; \psi\varphi \tag{5.31}$$

and $\rho = |\nabla h|$ on $\mathcal{E}_\lambda$ and

$$\theta|_{C_\lambda} \;=\; 0 \;,$$

we find for the $k=0$ term

$$\rho b e^{i\theta/\alpha}|_{C_\lambda} \;=\; \psi\varphi|\nabla h| \;. \tag{5.32}$$

Next we compute the $k=1$ term. Since

$$\theta \;=\; O\big((z-\sigma)^3\big) \;, \tag{5.33}$$

for $\sigma \in C_\lambda$, we have that

$$L(b\rho e^{i\theta/\alpha}) \;=\; L(b\rho) \qquad \text{on} \qquad C_\lambda\ . \tag{5.34}$$

Since $\hat{\chi}^{(k)}(0) = 0$ for $k = 1, 2$, we find

$$L(b\rho) \;=\; L(\psi a\rho) \qquad \text{at} \qquad t = 0\ .$$

Next, we use that

$$a \;=\; a_0 + O(\alpha)\ ,$$

where a_0 obeys the first of transport equations (5.7)–(5.8) and $O(\alpha)$ stands for a smooth, compactly supported symbol of order $O(\alpha)$ (see equation (5.6)). The last two equations yield

$$L(b\rho) \;=\; L(\psi a_0\rho) + O(\alpha) \tag{5.35}$$

at $t = 0$. Of course, this estimate remains valid after restriction to $\mathcal{E}_\lambda$ and integration over it. Next we use the transport equation for a_0

$$\partial_t a_0 + \partial_x S \cdot \partial_x a_0 + \frac{1}{2}\Delta_x S a_0 \;=\; 0 \tag{5.36}$$

and the initial condition

$$a_0|_{t=0} \;=\; \varphi\ . \tag{5.37}$$

These two relations imply

$$\partial_t a_0|_{t=0} \;=\; -\frac{1}{2}\Delta_x S|_{t=0}\varphi\ .$$

This together with $S|_{t=0} = x \cdot \xi$ gives

$$\partial_t a_0|_{t=0} \;=\; 0\ . \tag{5.38}$$

Now we need the explicit form of L . It is easy to check that

$$\phi''(\sigma)^{-1} \;=\; \begin{pmatrix} 0 & -\nabla h|\nabla h|^{-2} \\ -(\nabla h)^T|\nabla h|^{-2} & \xi \cdot \nabla W|\nabla h|^{-4}\nabla h \otimes \nabla h \end{pmatrix}$$

where $\nabla h \otimes \nabla h$ stands for the matrix $(\partial_{y_i} h \partial_{y_j} h)$. Plugging this into (5.28) gives

$$L \;=\; -2\frac{\nabla h}{|\nabla h|^2} \cdot \partial_y \partial_t + \frac{\xi \cdot \nabla W}{|\nabla h|^4} \langle (\nabla h \otimes \nabla h)\nabla, \nabla \rangle \;. \tag{5.40}$$

Using this expression together with (5.37) and (5.38), we find

$$L(\psi \rho a_0)\,\Big|_{t=0} \;=\; \frac{\xi \cdot \nabla W}{|\nabla h|^4} \langle (\nabla h \otimes \nabla h)\nabla, \nabla \rangle (\psi \varphi \rho) \;. \tag{5.41}$$

Combining equations (5.34), (5.35) and (5.41), we obtain

$$L(b\rho e^{i\theta/\alpha}) \;=\; \xi \cdot \nabla W j + O(\alpha) \tag{5.42}$$

on C_λ, where

$$j \;=\; |\nabla h|^{-4} \langle (\nabla h \otimes \nabla h)\nabla, \nabla \rangle (\psi \varphi \rho) \;. \tag{5.43}$$

Note now that

$$j(x, -\xi) \;=\; j(x, \xi) \tag{5.44}$$

and the same property holds for $|\nabla h|$ and h. Hence

$$\int_{\mathcal{E}_\lambda} (\xi \cdot \nabla W j |\nabla h|^{-1})_{\mathcal{E}_\lambda} dS_\lambda \;=\; 0 \;. \tag{5.45}$$

Plugging (5.32) and (5.42) into (5.27) and taking into account (5.45), we find (5.17).

6. Estimates of the Evolution

In this section we estimate the difference $U(t) - F(t)$, between the true evolution operator $U(t)$ and its approximation $F(t)$. After that, using estimates on $F(t)$, derived in the previous section, we estimate $U(t)$. The estimates on $U(t)$ obtained in this section are used in the next section in order to find asymptotic behaviour of the spectral projections $E(\lambda, H_\alpha)$. Our arguments follow closely those of [Chaz 1980]. Recall that $\varphi \in C_0^\infty\big(B(0,2) \times B(0,K)\big)$ is the cut-off function entering the construction of $F(t)$ and N is the order of approximation used in this construction (see eqn (5.6)).

Lemma 6.1. *Let $\varphi_1 \in C_0^\infty$ and be supported in $\{\varphi = 1\}$ and let $\operatorname{supp}\varphi_1$ be disjoint from $\operatorname{supp}(\nabla_x\varphi)$. Then*

$$\sup_{|t|\le T} \|\big(F(t) - U(t)\big)\phi_1\|_1 \ \le \ C\alpha^{N+1-d} \ , \tag{6.1}$$

where $\phi_1 = \varphi_1(x, D_x)$, provided T is sufficiently small.

Proof. Introduce

$$r \ \equiv \ e^{-iS/\alpha}(D_t - H)(e^{iS/\alpha}a) \ , \tag{6.2}$$

where S and a obey (5.4)–(5.8). Performing differentiations and using equations (5.4) and (5.7), we arrive at

$$r \ = \ \frac{1}{2}\alpha^{N+2}\Delta_x a_N \ . \tag{6.3}$$

Let

$$R(t)u \ = \ \alpha^{-d}\int\int e^{i(S - z\cdot\xi)/\alpha} r u dz d\xi \ . \tag{6.4}$$

Since a_N is smooth and compactly supported, we have

$$\sup_{|t|\le T} \|\nabla_x^n R(t)\|_1 \ \le \ C\alpha^{N+2-d-n} \tag{6.5}$$

where T is the time till which the Hamilton-Jacobi and transport equations were solved.

Now observe that, due to (6.2), $F(t)$ obeys

$$(D_t - H)F(t) \ = \ R(t) \ . \tag{6.6}$$

Moreover,

$$F(0) \;=\; \varphi(x, D_x)\;. \tag{6.7}$$

Consequently, the family $G(t) = F(t) - U(t)$ obeys the equation

$$(D_t - H)G(t) \;=\; R(t) \tag{6.8}$$

and

$$G(0) \;=\; -\bar{\phi}\;, \tag{6.9}$$

where $\bar{\phi} = \mathbf{1} - \varphi(x, D_x)$. Integrating out these equations, we obtain

$$G(t) \;=\; \frac{1}{\alpha i}\int_0^t U(t-s)R(s)ds - U(t)\bar{\phi}\;,$$

which together with (6.5) for $n = 0$ and the relation $\overline{\phi}\cdot\phi_1 = O(\alpha^M)$ for any M, which follows from $(1-\varphi)\cdot\varphi_1 = 0$, gives (6.1).

Theorem 6.2. *Let* $\varphi = 1$ *on* $B(0, \frac{3}{2}) \times B(0, K-1)$ *and let* $\nabla_x\varphi$ *be supported in* $|x| \geq \frac{3}{2}$. *Let* $K = 2(\sup\limits_{B(0,2)} W)_+^{\frac{1}{2}} + 3$ *and let* $\psi \in C_0^\infty\big(B(0,1)\big)$. *Then*

$$\begin{aligned} &\| \int \theta(t)\big(F(t) - U(t)\big)dt\psi\|_1 \\ &\leq C\alpha^{N-2d} \end{aligned} \tag{6.10}$$

with the constant independent of α , *provided* $\theta \in C_0^\infty([-T,T])$ *with* T *sufficiently small.*

Proof. In this proof we omit the argument t and replace the symbol $\int\limits_{-\infty}^{\infty} dt$ by $\int$. Let $\eta \in C_0^\infty\big(B(0, K - \frac{3}{2})\big)$ and $=1$ on $B(0, K-2)$. By (5.12)

$$\| \int \theta F \bar{\eta}(D_x)\|_1 \;\leq\; C\alpha^A\;, \tag{6.11}$$

where $\bar{\eta} = 1 - \eta$, for any $A \geq 0$. By lemma 6.1

$$\| \int \theta(F-U)\eta(D_x)\psi\|_1 \;\leq\; C\alpha^{N-d}\;. \tag{6.12}$$

Now we consider the term $\int \theta U \bar{\eta}(D_x)$. If $\check{\theta}^{\text{normal}}(\lambda) = \frac{1}{2\pi}\int e^{it\lambda}\theta(t)dt$ is the standard inverse Fourier transform of $\theta(t)$ (to distinguish from the α-Fourier transform used in the next section), then

$$\int \theta U \;=\; \check{\theta}^{\text{normal}}(-H_\alpha/\alpha)\ . \tag{6.13}$$

Since $|\check{\theta}^{\text{normal}}(\lambda)| \;\le\; C\langle\lambda\rangle^{-A}$ for any $A \ge 0$, we have that $\left(\frac{H_\alpha}{\alpha}\right)^A \check{\theta}^{\text{normal}}\left(-\frac{H_\alpha}{\alpha}\right)$ is bounded for any $M \ge 0$. On the other hand, for $\bar{g}(\lambda)$, smooth, bounded and $=0$ for $|\lambda| \le \frac{1}{2}$, $H_\alpha^{-M}\bar{g}(H_\alpha)$ is bounded for any $M \ge 0$. The last two relations together with (4.5) yield that

$$\|\int \theta U \bar{g}(H_\alpha)\psi\|_1 \;\le\; C\alpha^A \tag{6.14}$$

for any $A \ge 0$. Let $\bar{g}(\lambda) = 1$ for $|\lambda| \ge 1$ and set $g(\lambda) = 1 - \bar{g}(\lambda)$. By theorem 4.3 and by our choice of K we have

$$\|\psi(x)\bar{\eta}(D_x)g(H_\alpha)\|_1 \;=\; O(\alpha^A)$$

for any $A > 0$. This together with (6.14), implies

$$\|\psi\bar{\eta}(D_x)\int \theta U\|_1 \;=\; O(\alpha^A)$$

for any $A \ge 0$. This together with (6.11) and (6.12) yields (6.10).

Replacing in theorem 6.2 H_α by $H_\alpha - \lambda$ and remembering definition (5.13), we obtain

Corollary 6.3. *Let $\psi \in C_0^\infty\big(B(0,1)\big)$ and $\varphi(x,\xi) = \psi_1(x)\eta(\xi)$ in (5.8) with $\psi_1 = 1$ on* $\operatorname{supp}\psi$ *, $\eta \in C_0^\infty\big(B(0,K)\big)$ and $K \ge 2(\sup_{B(0,2)} W + \lambda)_+^{\frac{1}{2}} + 3$. Let $\hat{\chi}$ be a smooth function supported in a sufficiently small neighbourhood of $t = 0$. Then*

$$\begin{aligned}&|\operatorname{tr}\big(\psi\int \hat{\chi}(t)U(t)e^{it\lambda/\alpha}dt\big) - I(\lambda,\alpha)|\\ &\quad\le\ \text{const}\ \alpha^{N-d}\ ,\end{aligned}$$

where N is the same as in (5.6) and $I(\lambda,\alpha)$ is defined with the ψ,φ and $\hat{\chi}$ as above.

7. Estimates of the Local Traces

In this section we estimate $\operatorname{tr}\big(\psi(x)g(H_\alpha)\big)$, where $\psi \in C_0^\infty\big(B(0,1)\big)$ and g is a smooth function on $\setminus\{0\}$ with a compact support. Due to the presence of a cut-off function ψ we call such a trace a local trace. In our approach we express $g(H_\alpha)$ in terms of the evolution $U(t)$ and use the information about the latter derived in the previous section. Since we have a good control of $U(t)$ for $|t| \le T$ and $T = O(1)$ we can estimate smooth functions of H_α supported on the scale $O(\alpha)$ (uncertainty principle). Using this and a more or less standard Tauberian technique, we estimate non-smooth functions of H_α with an error term related to the degree of their non-smoothness. The main result of this section is theorem 7.1.

In what follows we will use the following α-dependent Fourier transform

$$\hat{f}(t) \;=\; \int e^{-it\lambda/\alpha} f(\lambda)d\lambda \;.$$

For the standard Fourier transform $(\alpha = 1)$ we reserve the notation

$$\hat{f}^{\text{normal}}(t) \;=\; \int e^{-it\lambda} f(\lambda)d\lambda \;.$$

We will use the following Fourier representation for functions of H_α:

$$g(H_\alpha) \;=\; \frac{1}{2\pi\alpha}\int \hat{g}(-t)U(t)dt \;, \tag{7.1}$$

where $\hat{g}(t)$ is the α-Fourier of $g(\lambda)$. $E(\lambda, H_\alpha)$ will stand for the spectral projection of H_α corresponding to the interval $(-\infty, \lambda)$. We define also the local counting function

$$e(\lambda,\psi,H_\alpha) \;=\; \operatorname{tr}\big(\psi E(\lambda,H_\alpha)\big) \;. \tag{7.2}$$

In the rest of this section we keep the subindex α at H_α in the theorems and omit it in the proofs.

Consider the following class of functions: $g(\lambda)$ is smooth on $\setminus\{0\}$, has a compact support and obeys for some $s \in [0,1]$, for some $\mu > 0$ and for all $\nu > 0$

$$b(\nu,g) \;\equiv\; \int_{|\sigma|\le 3\nu} |g'(\sigma)|d\sigma + \nu\int_{|\sigma|\ge\nu} |g''(\sigma)|d\sigma \;\le\; (M\nu)^s \;. \tag{7.3}$$

Let $b(g) = \sup\limits_{\nu>0}\big(\nu^{-s}b(\nu,g)\big)$. We begin with

Theorem 7.1. *Let* g *be as specified above with* $0 \leq s \leq 1$ *and* $M > 0$ *(see (7.3)). Let* $\psi \in C_0^\infty\big(B(0,1)\big)$ *and let* 0 *be a regular value of the function* h *restricted to* $\operatorname{supp}\psi \times {}^d$. *Then for* $\alpha \leq 1$

$$\begin{aligned} \operatorname{tr}\big(\psi g(H_\alpha)\big) \;&= \alpha^{-d}\int\!\!\int \psi(x) g\big(h(x,\xi)\big) dx d\xi \\ &\quad + O(b(g)\alpha^{s+1-d}) \; . \end{aligned} \tag{7.4}$$

Proof. Let χ be a symmetric function, $\chi(-\lambda) = \chi(\lambda)$ whose α-Fourier transform, $\hat{\chi}$, is smooth and obeys

$$\hat{\chi}(0) = 1 \qquad \text{and} \qquad \operatorname{supp}\hat{\chi} \subset [-T;T] \tag{7.5}$$

with $T \leq \tau$. (For the definition of τ see the paragraph after eqn (5.16).) Function χ will serve as a δ-approximation supported on the scale $O(\alpha)$. It is of the form $\chi(\lambda) = \frac{1}{\alpha}\chi_1\left(\frac{\lambda}{\alpha}\right)$, where χ_1 is a function whose standard (α-independent) Fourier transform satisfies (7.5). To probe different energies we use

$$\begin{aligned} \frac{1}{2\pi\alpha}\int \hat{\chi}(t) U(t) e^{i\lambda t/\alpha} dt \;&=\; \chi(\lambda - H_\alpha) \\ &=\; \chi * dE \; . \end{aligned} \tag{7.6}$$

This equation, Corollary 6.3 and Theorem 5.2 yield

$$\chi * de - de_0 \;=\; O(\alpha^{2-d}) \; , \tag{7.7}$$

at a non-critical value of h on $\operatorname{supp}\psi \times B(0,K)$. Here $K \geq 2(\sup\limits_{B(0,2)} W + \lambda)_+^{\frac{1}{2}} + 3$ and

$$e_0(\lambda,\psi,H_\alpha) \;=\; \alpha^{-d}\int\!\!\int_{h(x,\xi)\leq\lambda} \psi(x) dx d\xi \; . \tag{7.8}$$

Integrating (7.7) from $-\sup\limits_{B(0,1)} W - 1$ to λ and using theorem 4.9, we obtain

$$\chi * e - e_0 \;=\; O(\alpha^{2-d}) \; , \tag{7.9}$$

provided $(-\infty,\lambda)$ contains no critical values of h on $\operatorname{supp}\psi \times B(0,K)$. Note here that making an argument slightly longer we could use a special case of simple inequality (6.14) instead of the more sophisticated theorem 4.4.

Lemma 7.2. *Let χ and g be as above and let $\varphi(\lambda) = -g'(-\lambda)$. Then*

$$\varphi * (\chi * e - e) \;=\; O(\alpha^{1+s-d}) \;. \tag{7.10}$$

Proof. It suffices to prove (7.10) for $\psi \geq 0$. Let θ be a real smooth positive function with $\int \theta = 1$ whose α-Fourier transform $\hat\theta(t)$ is supported in $(-\tau, \tau)$. As before define θ_1 by $\theta(\lambda) = \frac{1}{\alpha}\theta_1\left(\frac{\lambda}{\alpha}\right)$. (4.41) implies

$$\theta * d_\lambda e \;\leq\; C\alpha^{-d} \;. \tag{7.11}$$

By the definition of θ, there are C and $\varepsilon > 0$ s.t.

$$C\alpha\theta(\lambda) \;\geq\; \eta(\lambda) - \eta(\lambda - \varepsilon\alpha) \;, \tag{7.12}$$

where $\eta(\lambda)$ is the characteristic function of the interval $(-\infty, 0]$. The last two inequalities together with (7.6) imply

$$e(\mu) - e(\mu - \varepsilon\alpha) \;\leq\; C\alpha^{1-d} \;. \tag{7.13}$$

Here and in the rest of the proof we use the shorthand $e(\mu) = e(\mu, \psi, H)$. Let $[\nu, \mu]$ contain no critical values of h. Decomposing the interval $[\nu, \mu]$ into $\frac{|\mu-\nu|}{\varepsilon\alpha}$ subintervals of the length $\varepsilon\alpha$ and applying (7.13) to each of these subintervals, we obtain

$$\begin{aligned} &|e(\mu) - e(\nu)| \\ &\qquad \leq\; C\alpha^{1-d}\left(\frac{|\mu-\nu|}{\alpha} + 1\right) \;. \end{aligned} \tag{7.14}$$

Let $e_\varphi = \varphi * e$. Then

$$\begin{aligned} &\varphi * (\chi * e - e) \\ &\quad =\; e_\varphi - \chi * e_\varphi \;. \end{aligned} \tag{7.15}$$

Since $\chi(\lambda)$ is even we can write $\chi * e_\varphi$ as

$$(\chi * e_\varphi)(\mu) \;=\; \int_{-\infty}^{\infty} \chi(\lambda)\big(e_\varphi(\mu+\lambda) + e_\varphi(\mu-\lambda)\big)d\mu \;. \tag{7.16}$$

Next, using that $\int \chi = 1$ and that χ is even, we find

$$\begin{aligned} & e_\varphi(\mu) - (\chi * e_\varphi)(\mu) \\ &= \int_0^\infty \chi(\lambda)\big(2e_\varphi(\mu) - e_\varphi(\mu+\lambda) - e_\varphi(\mu-\lambda)\big)d\lambda \ . \end{aligned} \tag{7.17}$$

Introduce the difference Laplacian

$$(\Delta_h f)(\mu) \ = \ 2f(\mu) - f(\mu+h) - f(\mu-h) \ ,$$

the difference gradient

$$(\nabla_h f)(\mu) \ = \ f(\mu+h) - f(\mu)$$

and the adjoint of the latter

$$(\nabla_h^* f)(\mu) \ = \ f(\mu-h) - f(\mu) \ .$$

Then

$$\begin{aligned} \Delta_h \ &= \ \nabla_h^* \nabla_h \\ &= \ \nabla_h \nabla_h^* \ . \end{aligned}$$

Using obvious properties of ∇_h , we obtain

$$\Delta_h e_\varphi \ = \ (\nabla_h^* \varphi) * \nabla_h e \ . \tag{7.18}$$

By (7.14)

$$|\nabla_h e| \ \le \ C\alpha^{1-d}\left(\frac{|h|}{\alpha} + 1\right) \ . \tag{7.19}$$

Next, we estimate

$$\begin{aligned} & \int_{-\infty}^\infty |\varphi(\sigma+h) - \varphi(\sigma)| d\sigma \\ & \le 2\int_{|\sigma|\le 3|h|} |\varphi(\sigma)| d\sigma \\ & \qquad + 2|h| \int_{|\sigma|\ge |h|} |\varphi'(\sigma)| d\sigma \ . \end{aligned}$$

Using condition (7.3), we obtain

$$\begin{aligned} & \int_{-\infty}^\infty |\varphi(\sigma+h) - \varphi(\sigma)| d\sigma \\ & \le 2b(|h|, g) \ . \end{aligned}$$

This together with relations (7.18) and (7.19) yields

$$|\Delta_h e_\varphi| \ \le \ C\alpha^{1-d}\left(\frac{|h|}{\alpha}+1\right)b(|h|,g) \ .$$

Remembering now (7.17) and using that $\chi(\lambda) = \frac{1}{\alpha}\chi_1\big(\frac{\lambda}{\alpha}\big)$, where χ_1 is the standard inverse Fourier transform of $\hat{\chi}$, we conclude that

$$\begin{aligned}
&|e_\varphi - \chi * e_\varphi| \\
&\le C\alpha^{1-d}\int_0^\infty \frac{1}{\alpha}\left|\chi_1\left(\frac{\lambda}{\alpha}\right)\right|\left(\frac{\lambda}{\alpha}+1\right)b(\lambda,g)d\lambda \\
&= C\alpha^{1-d+s}b(g) \ .
\end{aligned}$$

This inequality together with (7.15) yields (7.11).

Now observe that

$$\varphi * (\chi * e) \ = \ \chi * (\varphi * e)$$

and

$$\begin{aligned}
\varphi * e\big|_{\lambda=0} \ &= \ g_- * de\big|_{\lambda=0} \\
&= \ \mathrm{tr}\,\big(\psi g(H)\big) \ ,
\end{aligned}$$

where $g_-(\lambda) = g(-\lambda)$. Moreover, with e_0 defined in (7.9),

$$\begin{aligned}
\varphi * e_0\big|_{\lambda=0} \ &= \ g_- * de_0\big|_{\lambda=0} \\
&= \ \alpha^{-d}\int\int \psi(x)g\big(h(x,\xi)\big)dxd\xi \ .
\end{aligned}$$

These relations together with equations (7.3) and (7.10) and lemma 7.2 yield

Lemma 7.3. *Assume, in addition to conditions of theorem 7.1, that* $\operatorname{supp} g$ *contains no critical values of* h *restricted to* $\operatorname{supp}\varphi$. *Then (7.4) holds.*

Remark 7.4. *Lemma 7.3 would suffice for* $d > 1$ *due to a result of the next section removing the restriction on the critical points of* h *in this case.*

Results in the spirit of lemma 7.3 but in a smooth case were obtained in [Chaz 1980, HelffRob 1990, Hux 1988, Ivrii 1986, Rob 1987].

Now we estimate $\operatorname{tr}\big(\psi(x)g(H_\alpha)\big)$ in a different, more elementary way. The restrictions on g are stronger now (in particular, step functions $(s=0)$ are not allowed) and the result below is weaker than (7.4), however, it has no restrictions concerning critical points of h. Combining this result with lemma 7.3 we will arrive at theorem 7.1.

Theorem 7.5. *Let g be a smooth function obeying $|\partial^n g(\lambda)| \le C_n(1+\lambda_+)^{-d}\langle\lambda\rangle^{-n}$. Let $\psi \in {}^\infty_0\big(B(0,1)\big)$. Then*

$$\operatorname{tr}\big(\psi g(H_\alpha)\big) = \alpha^{-d}\int\int \psi(x) g\big(h(x,\xi)\big)dxd\xi + O(\alpha^{2-d}) \; . \tag{7.20}$$

Proof. Introduce an auxiliary potential $W_0(x)$ as $W_0 \in C_0^\infty({}^d)$ and $= W(x)$ in $B(0,2)$. Let $H_{0,\alpha} = -\frac{\alpha^2}{2}\Delta - W_0(x)$. Then by theorem 4.6

$$\|\psi\big(g(H_\alpha) - g(H_{0,\alpha})\big)\|_1 \le C\alpha^A \tag{7.21}$$

for any A. By a standard α-pseudo-differential Calculus $g(H_{0,\alpha})$ is an α-pseudo-differential operator with the symbol of the form

$$g(h_0) - \frac{1}{2}\alpha\xi\cdot\nabla W_0 g''(h_0) + \alpha^2 r_\alpha \tag{7.22}$$

where $h_0 = \frac{1}{2}|\xi|^2 - W_0(x)$ and the symbol r_α obeys

$$\int\int |\psi(x) r_\alpha(x,\xi)| dxd\xi \le C \tag{7.23}$$

uniformly in α. Writing out the trace in terms of the symbol of $\psi(x)g(H_{0,\alpha})$ and using the fact above, we obtain

$$\begin{aligned}\operatorname{tr}\psi g(H_{0,\alpha}) &= \alpha^{-d}\int\int \psi g(h_0) \\ &\quad - \frac{1}{2}\alpha^{1-d}\int\int \xi\cdot\nabla W_0 g''(h_0)dxd\xi + O(\alpha^{2-d}) \; .\end{aligned} \tag{7.24}$$

Since $h_0(x,-\xi) = h(x,\xi)$, we have

$$\int \xi\cdot\nabla W_0 g''(h_0)d\xi = 0 \; . \tag{7.25}$$

Equations (7.21), (7.24) and (7.25) and the relation $h_0 = h$ on $\operatorname{supp}\psi$ yield (7.20).

Remark 7.6. In the supplement we give a direct and elementary proof of (7.20).

We complete now the proof of theorem 7.1. Let g be the same as in theorem 6.1. We write it as

$$g \;=\; g_1 + g_2$$

where g_1 has the same properties as g with addition that it is supported in a small neighbourhood of 0 so that $\operatorname{supp} g_1$ contains no critical values of h restricted to $\operatorname{supp}\psi \times {}^d$ except, possibly, $\lambda = 0$, and $g_2 \in C_0^\infty$. Applying lemma 7.3 to g_1 and theorem 7.5 to g_2, we arrive at the result of theorem 7.1.

Remark 7.7. In order to obtain the next term in expansion (7.4) one would have to improve lemma 7.2. One way of doing this is by exercising a better control of τ, the maximal time during which the classical trajectories beginning in $B(0,1) \times {}^d$ neither hit one of the singularities nor return to their starting points. It is easy to trace the explicit dependence of the r.h.s. of (7.11) on τ. Namely, we have

$$\varphi * (\chi * e - e) \;=\; O\left(\alpha^{-d}\left(\frac{\alpha}{\tau}\right)^{1+s}\right) .$$

Thus if $\tau = O(\alpha^{-\varepsilon})$ for some $\varepsilon > 0$, one can obtain the second $-\alpha^{2-d}$-term in the expansion for $\operatorname{tr}\bigl(\psi g(H_\alpha)\bigr)$. An equation extending (7.22) to a higher order in which $g(\lambda)$ is replaced by $g(\lambda\alpha^{-\mu})$ shows that it suffices to study the classical trajectories in the energy interval $[-\alpha^\mu, 0]$ with $\mu < \frac{1}{6}$. (The latter condition is not sharp: the uncertainty principle suggests that it should suffice to take $\mu < 1$.)

8. Multiscale Analysis

The core of this section is a multiscale analysis which allows us to relax the condition in theorem 7.1 concerning critical values of the Hamiltonian h (or the potential $W(x)$) and to extend this theorem to singular potentials. There are three scales in the problem: the momentum scale β^{-1} determined by the quasiclassical parameter β entering the definition of the kinetic energy, the length scale $\ell(x)$ determined by the behaviour of the potential near critical points or near singularities and the energy scale, $f(x)^2$, determined by the size of potential. The first scale is constant while the other two depend on x. Scaling the coordinate and energy appropriately, we reduce the original problem to a model one, treated in the previous section, but with the effective quasiclassical parameter

$$\alpha_{\text{eff}}(x) \;=\; \frac{\beta}{\ell(x)f(x)} \ ,$$

which depends on all the scales. Applying to the latter problem theorem 6.1 and rescaling the result back we obtain the desired quasiclassical expansion for the original problem. One of the consequences of this is a quasiclassical expansion for a singular potential outside a small neighbourhood of singularities. Decoupling of the latter neighbourhood and estimation within it is done in the next two sections, respectively.

We consider the Schrödinger operator

$$K_\beta \;=\; -\frac{1}{2}\beta^2\Delta - \phi(x) \quad \text{on} \quad {}^d \ .$$

Its symbol is denoted by

$$k(x,\xi) \;=\; \frac{1}{2}|\xi|^2 - \phi(x) \ .$$

We assume that $\phi(x)$ is real and obeys the Kato inequality:

$$||\phi u|| \;\leq\; \varepsilon||\Delta u|| + \frac{C}{\varepsilon^2}||u|| \tag{8.1}$$

for all $u \in \mathcal{D}(\Delta)$ and for all $\varepsilon > 0$ and with C independent of ε and u.

We impose, in addition, the following conditions on the potentials $\phi(x)$: there are differentiable functions $\ell(x)$ and $f(x)$ obeying

$$\ell(x) > 0 \quad \text{a.e. and} \quad |\nabla \ell(x)| \leq L \tag{8.2}$$

for some $L > 0$ and

$$f(x) > 0 \quad \text{a.e. and } c^{-1} \leq \frac{f(x)}{f(y)} \leq c \quad \text{on } B\big(y, \ell(y)\big) \tag{8.3}$$

for $1 < c < \infty$, i.e. f is slowly varying on the scale of ℓ, and s.t.

$$|\partial^\nu \phi(x)| \ \leq \ C_\nu f(x)^2 \ell(x)^{-|\nu|} \ . \tag{8.4}$$

In the rest of this section $\int\int$ stands for the (x,ξ)-integral over the phase-space (remember the normalization $d\xi = (2\pi)^{-d}\times$ Lebesgue measure).

Theorem 8.1. *Assume conditions (8.1)–(8.4) are obeyed and let* ψ *be smooth and obey* $|\partial^\nu \psi(x)| \leq C_\nu \ell(x)^{-|\nu|}$ *for any* ν. *Let* g *be smooth on* $\backslash\{0\}$ *and satisfy (7.3) and* $|g(\lambda)| \leq C(-\lambda)_+^s$ *for some* $s \in [0,1]$. *Then*

$$\begin{aligned} &|\mathrm{tr}\,\big(\psi g(K_\beta)\big) - \beta^{-d} \int\int \psi g(k)| \\ &\leq \ C\beta^{2s} \int_{\Omega_\psi} \max\Big[\Big(\frac{\beta}{f(x)\ell(x)}\Big)^{\rho - s - d}, 1\Big] \ell(x)^{-2s-d} dx \ , \end{aligned} \tag{8.5}$$

where $\Omega_\psi = \bigcup\limits_{y \in \mathrm{supp}\,\psi} B\big(y, \ell(y)\big)$ *and where with* C *independent of* β. *Here* $\rho = 1$ *if either* $d \geq 2$ *or* $d = 1$ *and* ϕ *obeys*

$$|\phi(x)| + \ell(x)|\nabla\phi(x)| \ \geq \ \varepsilon f(x)^2 \tag{8.6}$$

on $\{x \mid \ell(x) f(x) \geq \beta\}$ *and with some* $\varepsilon > 0$ *independent of* β *and* $\rho = \frac{1}{2}$ *otherwise.*

Proof. First we demonstrate this statement under the additional restrictions that ψ is supported in $\{x \mid \ell(x) f(x) \geq \beta\}$ and that (8.6) holds on $\Omega_1 = \{x \mid \ell(x) f(x) \geq \delta\beta\}$ for some sufficiently small $\delta > 0$ (e.g. $\delta = c^{-1}(1-L)$ after choosing $L < 1$). Then we use the obtained result to remove this restriction.

Note first that by rescaling $\ell(x)$ we can assume $L < \frac{1}{2}$ in (8.2). In this case (8.2) implies

$$\frac{1}{1+L}\ell(y)^{-1} \ \le\ \ell(x)^{-1} \ \le\ \frac{1}{1-L}\ell(y)^{-1} \quad \text{on} \quad B\big(y,\ell(y)\big) \ . \tag{8.7}$$

Next, using (8.3), we derive from (8.4) and (8.6)

$$|\partial^\gamma \phi(x)| \ \le\ C_\gamma f(y)^2 \ell(y)^{-|\gamma|} \tag{8.8}$$

and

$$|\phi(x)| + \ell(y)|\nabla\phi(x)| \ \ge\ \varepsilon_1 f(y)^2 \tag{8.9}$$

for some $\varepsilon_1 > 0$ independent of y and β, for all x in $B\big(y,\ell(y)\big) \cap \Omega_1$. Next, we need the following

Lemma 8.2. *Assume that for some constants $f, \ell > 0$, s.t. $f\ell \ge \beta$, $\phi(x)$ obeys on $B(y, 2\ell)$ the estimates*

$$|\partial^\gamma \phi(x)| \ \le\ C_\gamma f^2 \ell^{-|\gamma|} \tag{8.10}$$

and

$$|\phi(x)| + \ell|\nabla\phi(x)| \ \ge\ \varepsilon f^2 \tag{8.11}$$

for some $\varepsilon > 0$. Let $\psi \in C_0^\infty\big(B(y,\ell)\big)$ with $|\partial^\gamma\psi| \le C_\gamma \ell^{-|\gamma|}$. Then

$$\begin{aligned} &|\mathrm{tr}\,\big(\psi g(K_\beta)\big) - \beta^{-d} \int\!\!\int \psi g(k)| \\ &\qquad \le\ C\beta^{s+1-d}\ell^{d-s-1}f^{s+d-1} \ , \end{aligned} \tag{8.12}$$

where C depends only on the C_γ 's above.

Proof. The idea of the proof is to scale the given problem to one in the unit ball and with a potential whose bounds are independent of f and ℓ. To this end we define the unitary transformation

$$U(\ell): \ \ \psi(x) \ \to\ \ell^{\frac{d}{2}}\psi(y+\ell x) \ ,$$

scaling x into ℓx, and use it to map K_β into

$$U(\ell)K_\beta U(\ell)^{-1} \;=\; \ell^{-2}\beta^2 D_x^2 - \phi(y+\ell x)\ .$$

Introduce the new potential

$$W(x) \;=\; f^{-2}\phi(y+\ell x)\ ,$$

the new quasiclassical parameter

$$\alpha \;=\; \frac{\beta}{f\ell} \tag{8.13}$$

and the new Schrödinger operator

$$H_\alpha \;=\; -\frac{1}{2}\alpha^2\Delta - W(x)\ .$$

Note that the new Schrödinger operator is related to the original one as

$$U(\ell)K_\beta U(\ell)^{-1} \;=\; f^2 H_\alpha \quad \text{with} \quad \alpha = \frac{\beta}{f\ell}\ . \tag{8.14}$$

Moreover, differentiating the new potential

$$\partial^\gamma W(x) \;=\; f^{-2}\ell^{|\gamma|}(\partial^\gamma\phi)(\ell x)$$

and using estimate (8.10), we find

$$|\partial^\gamma W(x)| \;\le\; C_\gamma \qquad \text{on} \qquad B(0,2)$$

with C_γ independent of f and ℓ. Moreover, we derive from (8.11) that

$$|W(x)| + |\nabla W(x)| \;\ge\; c \tag{8.15}$$

on $B(0,2)$ for some $c > 0$. Of course, W obeys the Kato inequality (with a constant depending on f and ℓ).

Next, due to (8.14)

$$g(f^2 H_\alpha) \;=\; U(\ell)g(K_\beta)U(\ell)^{-1}\ . \tag{8.16}$$

Using that $U(\ell)\psi U(\ell)^{-1}$ is the multiplication operator by $\varphi(x) \equiv \psi(\ell x)$ and using the invariance of the trace under similarity transformations, we obtain

$$\operatorname{tr}\big(\psi g(K_\beta)\big) \;=\; \operatorname{tr}\big(\varphi g(f^2 H_\alpha)\big) \tag{8.17}$$

with $\alpha = \beta / f\ell$.

Observe now that $\varphi \in C_0^\infty\big(B(0,1)\big)$, $|\partial^\gamma \varphi| \le C_\gamma$ independently of ℓ and 0 is not a critical value of $h = \frac{1}{2}|\xi|^2 - W(x)$ on $\operatorname{supp}\varphi \times {}^d$. Since $g(f^2\lambda)$ obeys (7.3), theorem 7.1 with $g(\lambda)$ replaced by $g(f^2\lambda)$ is applicable to H_α and it yields

$$\begin{aligned} &|\operatorname{tr}\big(\varphi g(f^2 H_\alpha)\big) - \alpha^{-d} \int\!\!\int \varphi g(f^2 h)| \\ &\quad \le\; C f^{2s} \alpha^{s+1-d} \;, \end{aligned} \tag{8.18}$$

where we have used that $b(g_f) = f^{2s} b(g)$ with $g_f(\lambda) = g(f^2\lambda)$. Remembering that in the first case (8.16) and the relation $\int\!\int \varphi(x) g(f^2 h) = 0$ yield an even stronger estimate we conclude that (8.18) holds in both cases.

Substituting (8.18) into (8.17) and using that $\alpha^{-d}\int\!\int \varphi g(f^2 h) = \beta^{-d} \int\!\int \psi g(k)$, we arrive at (8.11).

Now we return to the proof of theorem 8.1 and recall that we have shown that ϕ obeys (8.8) and (8.9) on $B\big(y, \ell(y)\big)$. Hence lemma 8.2 is applicable on this ball and with $f = f(y)$ and $\ell = \ell(y)$, provided $\ell(y) f(y) \ge \beta$, which gives

$$\begin{aligned} &|\operatorname{tr}\big(\psi_y g(K_\beta)\big) - \beta^{-d} \int\!\!\int \psi_y g(k)| \\ &\quad \le\; C \beta^{s+1-d} f(y)^{d-1} \ell(y)^{d-s-1} \;, \end{aligned} \tag{8.19}$$

where $\psi_y \in C_0^\infty\Big(B\big(y, \ell(y)\big)\Big)$ and is s.t. (8.6) holds on $\operatorname{supp}\psi_y \times {}^d$. Using now (8.3) and (8.7) in order to estimate the r.h.s. of (8.19), we obtain

$$\begin{aligned} &|\operatorname{tr}\big(\psi_y g(K_\beta)\big) - \beta^{-d} \int\!\!\int \psi_y g(k)| \\ &\quad \le\; C \beta^{s+1-d} \int_{B\left(y,\ell(y)\right)} f(x)^{d+s-1} \ell(x)^{-s-1} dx \;. \end{aligned} \tag{8.20}$$

Finally, we cover $\operatorname{supp}\psi$ with balls $B\big(y,\ell(y)\big)$, $y \in \operatorname{supp}\psi$. Since $\ell(x)$ is slowly varying these balls can be chosen so as to have finite intersection property, i.e. there is a constant M_1 s.t. the intersection of more than M_1 balls is empty. Moreover, there is a partition of unity $\{j_y\}$ associated with this covering s.t. j_y is supported in $B\big(y,\ell(y)\big)$, $\sum j_y = 1$ on $\operatorname{supp}\psi$ and $\partial^\alpha j_y = O\big(\ell(y)^{-|\alpha|}\big)$ (see [Hörm I. theorem 1.4.10]). Using this partition of unity, we decompose

$$\psi \;=\; \sum \psi_y$$

with ψ_y supported in $B\big(y,\ell(y)\big)$ and obeying $\partial^\nu \psi_y \;=\; O\big(\ell(y)^{-|\nu|}\big)$. Using now (8.21) for each of the ψ_y's, we obtain (8.6) with $\rho = 1$. Note that additional restriction (8.6) is equivalent to the condition that 0 is not a critical value of the rescaled Hamiltonian h on $B(0,2) \times {}^d$.

Thus we have proven theorem 8.1 with $r = 1$ and with the additional restriction (8.6) on Ω_1. Now we use this result in order to strengthen the key theorem 7.1 used in the proof of this result. Namely, for $d \geq 2$ we remove from the latter theorem the condition that 0 is not a critical value of h restricted to $B(0,1) \times {}^d$, which in turn will allow us to remove this condition from the proof of (8.5) given above!

In the one-dimensional case by the order of a critical point x_0 of ϕ we understand the order of the first non-vanishing derivative of ϕ at x_0 minus 1.

Theorem 8.3. *Let W obey the conditions given in the beginning of section 4. Let $\psi \in C_0^\infty\big(B(0,1)\big)$ and let g be the same as in theorem 8.1. Then*

$$\begin{aligned} \operatorname{tr}\big(\psi g(H_\alpha)\big) - \alpha^{-d} \int\!\!\int \psi g(h) \\ \;=\; O\big(\alpha^{s+1-d}\varphi(\alpha)\big)\,, \end{aligned} \tag{8.21}$$

where $\varphi(\alpha) \equiv 1$ if either $d \geq 2$ or $d = 1$ and W has no critical points in $B(0,1) \cap W^{-1}(\operatorname{supp} g)$, $\varphi(\alpha) = |\ln\alpha|$ if $d = 1$ and $n = 1$ and $\varphi(\alpha) = \alpha^{-\frac{1}{2}}$ if $d = 1$ and $\infty \geq n \geq 2$. Here n is the maximal order of critical points of W on $B(0,1) \cap W^{-1}(0)$.

Proof. We define the length scale as

$$\begin{aligned} \ell(x) &= M_1^{-1}|\nabla h||_{h=0} \\ &= \frac{1}{M_1}(|W| + |\nabla W|^2)^{\frac{1}{2}} , \end{aligned} \tag{8.22}$$

where M_1 is given by

$$\begin{aligned} M_1 &= 1 + 2\sup_x \|\text{Hessian } W(x)\| \\ &\geq 2 \sup_x |\nabla(|\nabla h|\big|_{h=0})| . \end{aligned}$$

Since $\ell(x) \leq \text{const}$ on $B(0,2)$, we have that

$$|\partial^\gamma W(x)| \leq C_\gamma \ell^{2-|\gamma|} .$$

This forces us to set the energy scale to be

$$f(x) = \ell(x) .$$

The definition of $\ell(x)$ and $f(x)$ implies that $W(x)$ obeys (8.2)–(8.4) and (8.6) with those $f(x)$ and $\ell(x)$. We have shown above that under these restrictions (8.5) with $r = 1$ is true, which in the present case yields

$$\begin{aligned} &|\text{tr}\big(\psi g(H_\alpha)\big) - \alpha^{-d} \int\int \psi g(h)| \\ &\leq C\alpha^{s+1-d} \int_{\Omega_\psi} \ell(x)^{d-2} dx \end{aligned} \tag{8.23}$$

for any $\psi \in C_0^\infty$ supported in

$$\begin{aligned} &\{f(x)\ell(x) \geq 2\alpha\} \\ &= \{\ell(x) \geq \sqrt{2\alpha}\} . \end{aligned}$$

Now we consider

$$\begin{aligned} &\{f(x)\ell(x) \leq 2\alpha\} \\ &= \{\ell(x) \leq \sqrt{2\alpha}\} . \end{aligned} \tag{8.24}$$

On this domain we pick the length and energy scales to be $\sqrt{\alpha}$ and α, respectively. Consider H_α on the ball $B(y, \sqrt{\alpha})$. Scaling

$$x \to y + \sqrt{\alpha}x$$

maps H_α into $\alpha\widetilde{H}$, where

$$\widetilde{H} \ = \ -\frac{1}{2}\Delta - \widetilde{W}(x)$$

with

$$\widetilde{W}(x) \ = \ \frac{1}{\alpha}W(y+\sqrt{\alpha}x)$$

obeying (8.16) on $B(0,1)$. Then theorem 7.1 with $\alpha = 1$ and with $g(\lambda)$ replaced by $g(\alpha\lambda)$ implies

$$\mathrm{tr}\left(\psi g(\alpha\widetilde{H})\right) \ - \ \int\int \psi g(\alpha\tilde{h}) \ = \ O(\alpha^s) \ ,$$

where $\tilde{h} = |\xi|^2 - \widetilde{W}(x)$, provided $\psi \in C_0^\infty\big(B(0,1)\big)$. (This is a trivial estimate if $g(\alpha\lambda) = \alpha^s g(\lambda)$ for $\alpha > 0$.) Rescaling this back to the original variables and using that, as above,

$$\mathrm{tr}\left(\psi g(\alpha\widetilde{H})\right) \ = \ \mathrm{tr}\left(\varphi g(H_\alpha)\right)$$

and

$$\int\int \psi g(\alpha\tilde{h}) \ = \ \alpha^{-d}\int\int \varphi g(h) \ ,$$

where $\varphi(x) = \psi\left(\frac{x-y}{\sqrt{\alpha}}\right)$, we obtain

$$\begin{aligned} &\mathrm{tr}\left(\varphi g(H_\alpha)\right) - \alpha^{-d}\int\int \varphi g(h) \\ &\quad = \ O(\alpha^s) \ . \end{aligned} \tag{8.25}$$

Now let

$$\ell_1(x) \ = \ \max\left(\ell(x), \sqrt{\alpha}\right) \ .$$

Then (8.25) can be rewritten as

$$\begin{aligned} &|\mathrm{tr}\left(\varphi g(H_\alpha)\right) - \alpha^{-d}\int\int \varphi g(h)| \\ &\quad \le \ C\alpha^{1+s-d}\int_{B(y,3\ell_1(y))} \ell_1(x)^{d-2}dx \ , \end{aligned} \tag{8.26}$$

provided φ is supported in $B\big(y,\ell_1(y)\big)$ and $B\big(y,3\ell_1(y)\big)$ lies in (8.24). On the other hand equation (8.23) and the observation that $\Omega_\varphi \subset B\big(y,3\ell_1(y)\big)$ for $\varphi \in C_0^\infty\big(B(y,3\ell(y)\big)$ imply (8.26) for any ball $B\big(y,3\ell_1(y)\big)$ lying in

$$\{x|\ell(x) \ \ge \ \sqrt{\alpha}\} \ .$$

Thus (8.26) holds for any ball $B\big(y, 3\ell_1(y)\big)$ (provided φ is supported in $B\big(y, \ell_1(y)\big)$ and obeys the corresponding estimates). Using, as above, a partition of unity associated with the length scale $\ell_1(x)$, we derive

$$\begin{aligned} &|\mathrm{tr}\,\big(\psi g(H_\alpha)\big) - \alpha^{-d}\int\int \psi g(h)| \\ &\quad\le\ C\alpha^{s+1-d}\int_{B(0,3)} \ell_1(x)^{d-2}dx \end{aligned} \tag{8.27}$$

for any $\psi \in C_0^\infty\big(B(0,1)\big)$ and with C independent of α and of $|\nabla h|^{-1}$. For $d \ge 2$, the integrand on the r.h.s. is bounded. For $d = 1$ it is $O\big((|x - x_0| + \sqrt{\alpha})^{-1}\big)$, if the order of the critical point x_0 is equal to 1 and is $O(\alpha^{-\frac{1}{2}})$ otherwise. Hence the r.h.s. of (8.27) can be bounded by const $\alpha^{s+1-r}\varphi(\alpha)$ and this inequality can be extended to $\Omega = B(0,1)$. This yields (8.21).

Now redoing the above proof of (8.5) but using theorem 8.3 instead of theorem 7.1 we conclude that (8.5) holds under the conditions of theorem 8.1 without additional restriction (8.6) in the $d \ge 2$ case, provided ψ is supported in $\{x \mid f(x)\ell(x) \ge \beta\}$.

Now we analyze the region $\{x \mid f(x)\ell(x) \le \frac{1}{2}\beta\}$.

Theorem 8.4. *Assume ϕ obeys (8.1)–(8.4). Let $C\lambda_-^s \le g(\lambda) \le 0$ for $0 \le s \le 1$. Let ψ be a smooth and bounded function supported in $\{x \mid f(x)\ell(x) \le \beta\}$. Then*

$$|\mathrm{tr}\big(\psi g(K_\beta)\big)|\ \le\ C\beta^{2s}\int_{\Omega_\psi} \ell(x)^{-2s-d}dx\ . \tag{8.28}$$

Proof. Denote $g_s(\lambda) = \lambda_-^s$. Without the restriction on generality we can assume $\psi \ge 0$ and $|\nabla\ell(x)| \le \frac{1}{2}$. $\psi \ge 0$ implies that

$$C\,\mathrm{tr}\big(\psi g_s(K_\beta)\big)\ \le\ \mathrm{tr}\big(\psi g(K_\beta)\big)\ \le\ 0\ .$$

Let y obey $f(y)\ell(y) \le \beta$. Let $\varphi \in C_0^\infty\big(B(y,\ell)\big)$, where $\ell = \ell(y)$, and satisfy $|\partial^\nu\varphi(x)| \le C_\nu\ell^{-|\nu|}$. Rescaling the problem as $x \to y + \ell x$, we obtain

$$\begin{aligned} &\mathrm{tr}\,\varphi(x)g_s(K_\beta) \\ &= \beta^{2s}\ell^{-2s}\mathrm{tr}\,\varphi_1(x)g_s(H)\ , \end{aligned} \tag{8.29}$$

where $\varphi_1(x) = \varphi(y + \ell x)$ and $H = -\frac{1}{2}\Delta - \phi_1(x)$ with

$$\phi_1(x) \;=\; \beta^{-2}\ell^2\phi(y + \ell x)\ . \tag{8.30}$$

Note that $\varphi_1 \in C_0^\infty\big(B(0,1)\big)$ and obey $|\partial^\nu \varphi_1| \le C_\nu$. Moreover, estimates (8.4) on $\phi(x)$ and inequality $\beta^{-1} f\ell \le 1$ imply that $\phi_1(x)$ obeys

$$|\partial^\nu \phi_1(x)| \;\le\; C_\nu$$

on $B(0,2)$. for a fixed $\delta > 0$. Hence, e.g. by theorem 4.10,

$$|\mathrm{tr}\, \varphi_1(x) g_s(H)| \;\le\; C\ ,$$

This together with (8.29) and (8.30) yields

$$\begin{aligned} |\mathrm{tr}\, \varphi(x) g(K_\beta)| \;&\le\; C\beta^{2s}\ell^{-2s} \\ &\le\; C_1\beta^{2s}\int_{B(y,\ell)} \ell(x)^{-2s-d}dx\ . \end{aligned}$$

Covering $\mathrm{supp}\,\psi$ by balls $B\big(y, \ell(y)\big)$ with $y \in \mathrm{supp}\,\psi$ and proceeding as in the proof of theorem 8.1, we arrive at (8.29).

In the classically forbidden region estimate (8.5) can be considerably improved.

Theorem 8.5. *Assume $\phi(x)$ obeys (8.1)–(8.4). Let ψ be a bounded function and let $g(\lambda)$ satisfy $|g(\lambda)| \le C(-\lambda)_+^s\langle\lambda\rangle^m$ for some m and $s \ge 0$ and let $\sup\limits_{\Omega_\psi}(f^{-2}\phi) < 0$. Then*

$$|\mathrm{tr}\ \psi(x) g(K_\beta)| \;\le\; C\int_{\Omega_\psi}\Big(\frac{\beta}{f(x)\ell(x)}\Big)^A f(x)^{2s}\langle f(x)\rangle^{2m}\ell(x)^{-d}dx \tag{8.31}$$

for any $A \ge 0$. Here, recall, Ω_ψ is defined in theorem 8.1.

Proof. Let $z \in \mathrm{supp}\ \psi$, $\ell = \ell(z)$ and $f = f(z)$ and let $\varphi \in C_0^\infty\big(B(y, \frac{1}{2}\ell)\big)$ and obey $|\partial^\nu\varphi(x)| \le C_\nu\ell^{-|\nu|}$ rescaling $x \to z + \ell x$ and energy $\to f^{-2}\ \times$ energy maps K_β into $f^2 H_\alpha$, where

$$H_\alpha \;=\; -\frac{\alpha^2}{2}\Delta_x - \phi_0(x)\ ,$$

with $\alpha = \frac{\beta}{f\ell}$ and $\phi_0(x) = f^{-2}\phi(z+\ell x)$. Observe that $|\partial^\nu \phi_0(x)| \le C_\nu$ on $B(0,2)$. Since the trace is invariant under similarity transformations, we have

$$\mathrm{tr}\ \varphi(x) g(K_\beta) \ = \ \mathrm{tr}\ \varphi_0(x) g(f^2 H_\alpha)\ , \tag{8.32}$$

where $\varphi_0 \in C_0^\infty\big(B(0,\frac{1}{2})\big)$ and obey $|\partial^\nu \varphi_0(x)| \le C_\nu$.

By the restriction on $g(\lambda)$ we have that $|g(f^2\lambda)| \le C f^{2s}\langle f\rangle^{2m}(-\lambda)_+^s\langle\lambda\rangle^m$. Hence there is a function $\widetilde{g}(\lambda)$ supported in $(-\infty, \sup\limits_{B(0,1)} \phi_0)$ and obeying $|\partial^n \widetilde{g}(\lambda)| \le C_n\langle\lambda\rangle^{m-n}$ and $\widetilde{g}(\lambda) \ge f^{-2s}\langle f\rangle^{-2m}|g(f^2\lambda)|$. Hence by a property of trace norms (see [Reed Sim II, p. 42])

$$\begin{aligned} &|\mathrm{tr}\ \varphi_0(x) g(f^2 H_\alpha)| \\ &\le f^{2s}\langle f\rangle^{2m}|\mathrm{tr}\ \varphi_0(x)\widetilde{g}(H_\alpha)|\ . \end{aligned} \tag{8.33}$$

Applying theorem 4.8 (see Remark 4.9b) to $\mathrm{tr}\ \varphi_0(x)\widetilde{g}(H_\alpha)$, we obtain

$$\mathrm{tr}\ \varphi_0(x)\widetilde{g}(H_\alpha) \ = \ O(\alpha^A) \tag{8.34}$$

for any $A \ge 0$. Remembering (8.32) and (8.33) and remembering that $\alpha = \frac{\beta}{f\ell}$, we find

$$|\mathrm{tr}\ \varphi(x) g(K_\beta)| \ \le \ C\Big(\frac{\beta}{f\ell}\Big)^A f^{2s}\langle f\rangle^{2m}\ . \tag{8.35}$$

Now, like in the end of the proof of theorem 8.1, covering $\mathrm{supp}\ \psi$ by the balls $B\big(z,\ell(z)\big)$ with $z \in \mathrm{supp}\ \psi$, associating with this covering a partition of unity, splitting $\mathrm{tr}\ \psi g(K_\beta)$ with the help of this partition of unity and applying (8.32) to each of the resulting sum, we obtain (8.28).

Remark 8.6. Theorem 8.5 can be derived from a natural generalization of theorem 8.1 to arbitrary $s \ge 0$. This generalization expresses $\mathrm{tr}\ \psi g(K_\beta)$ as a sum of $[s]+1$ Weyl-type local terms, as given by a standard quasiclassical pseudo-differential calculus, plus the error of order $O(\alpha^{1+s-d})$, where $\alpha = \frac{\beta}{f\ell}$. In the classically forbidden region the local, Weyl-type terms vanish, so the result follows.

We combine now theorems 8.1 and 8.5.

Theorem 8.7. *Assume the conditions of theorem 8.1 are obeyed and let* ψ, Ω_ψ *and let* ρ *be the same as in theorem 8.1. Then for any* $A \geq 0$ *and any* $\mu \leq 0$

$$\begin{aligned} &|\mathrm{tr}\, \psi g(K_\beta - \mu) - \beta^{-d} \int\int \psi g(k-\mu)| \\ &\leq C\beta^{2s} \int_{\Omega_\psi \cap Q_{\frac{1}{2}\beta}} \Big(\frac{\beta}{f\ell}\Big)^{\rho-s-d} \ell^{-2s-d} dx \\ &\quad + C\beta^{2s} \int_{\Omega_\psi \cap Q^c_\beta} \min\Big(\frac{\beta/\sqrt{-\mu}}{\ell}, 1\Big)^A \ell^{-2s-d} dx\ , \end{aligned} \tag{8.36}$$

where C *depends only on* d *and on the constants in (8.3) and (8.4) and where* $Q_\beta = \{x \mid f(x)\ell(x) \geq \beta\}$ *and* $Q^c_\beta = {}^d\backslash Q_\beta$ *.*

Proof. Let $f_1(x)$ be a positive function satisfying eqn (8.3) and obeying $f_1(x) \geq f(x)$. Define the domains

$$R_1 = \Big\{x \mid \phi(x) \geq -\frac{\mu}{3} - 3C_0 c^3 f_1(x)^2\Big\}$$

and

$$R_2 = \Big\{x \mid \phi(x) \leq -\frac{1}{2}\mu - 2C_0 c^3 f_1(x)^2\Big\}\ ,$$

where C_0 is the constant entering (8.4) for $\nu = 0$ and c is the same as in (8.3). We begin with

Lemma 8.8. *With the conditions and notation of theorem 8.1 we have for any* A *and for any* $\mu \leq 0$

$$\begin{aligned} &|\mathrm{tr}\ \psi g(K_\beta - \mu) - \beta^{-d} \int\int \psi g(k-\mu)| \\ &\leq C\beta^{2s} \int_{\Omega_\psi \cap R_1} \max\Big[\Big(\frac{\beta}{f_1(x)\ell(x)}\Big)^{\rho-s-d}, 1\Big] \ell(x)^{-2s-d} dx \\ &\quad + C\beta^{2s} \int_{\Omega_\psi \cap R_2} \Big(\frac{\beta}{f_1(x)\ell(x)}\Big)^A \ell(x)^{-2s-d} dx\ . \end{aligned} \tag{8.37}$$

Proof. On R_1 the potential $\phi(x) + \mu$ obeys (8.1)–(8.4) but with $f(x)$ replaced by $f_1(x)$. Hence theorem 8.1, with $f_1(x)$ instead of $f(x)$, is applicable to $K_\beta - \mu$ and yields that the l.h.s. of (8.37) is bounded by

$$C\beta^{2s} \int_{\Omega_\psi} \max\Big[\Big(\frac{\beta}{f_1(x)\ell(x)}\Big)^{\rho-s-d}, 1\Big] \ell(x)^{-2s-d} dx$$

for any ψ supported in R_1 .

On R_2 the potential $\phi(x)+\mu$ obeys (8.1)–(8.4) but with $f(x)$ replaced by $\max\big(f_1(x),\sqrt{-\mu}\big)$. Let $R_3=\{x \mid \phi(x)\le -\frac{1}{2}\mu - C_0 c f_1(x)^2\}$. Using that $\phi(x)\le \phi(y)+|\phi(x)-\phi(y)|$ and that $|\phi(x)-\phi(y)|\le C_0 c f(x)^2$ on $B\big(y,\ell(y)\big)$, we derive that $\Omega_\psi\subset R_3$, provided that $\operatorname{supp}\psi\subset R_2$. Furthermore, since

$$\sup_{R_3}\big\{\big[\max\big(f_1(x),\sqrt{-\mu}\big)\big]^{-2}\big(\phi(x)+\mu\big)\big\} \ \le\ -\min\Big(\frac{1}{2},cC_0\Big)\ ,$$

we have that

$$\operatorname{supp} g\subset\Big(-\infty,-\sup_{R_3}\big\{\big[\max\big(f_1(x),\sqrt{-\mu}\big)\big]^{-2}\big(\phi(x)+\mu\big)\big\}\Big)\ .$$

Hence theorem 8.4 with $f(x)$ replaced by $\max\big(f_1(x),\sqrt{-\mu}\big)$ is applicable to $K_\beta-\mu$ and yields that for any $\mu\le 0$ and for any A

$$|\operatorname{tr}\psi g(K_\beta-\mu)|\ \le\ C\beta^{2s}\int_{\Omega_\psi}\Big(\frac{\beta}{f_1(x)\ell(x)}\Big)^A\ell(x)^{-2s-d}dx$$

provided ψ is supported in R_2 and is bounded. Since, moreover, $\int\int\psi g(k-\mu)=0$ for such ψ 's, we conclude that the l.h.s. of (8.37) is bounded by

$$C\beta^{2s}\int_{\Omega_\psi}\Big(\frac{\beta}{f_1(x)\ell(x)}\Big)^A\ell(x)^{-2s-d}dx$$

for any A , provided ψ is bounded and is supported in R_2 . This together with the conclusion of the previous paragraph yields (8.37).

Now we return to the proof of theorem 8.7. We pick up $f_1(x)$ as

$$f_1(x)\ =\ f(x)+\frac{\sqrt{-\mu}}{\sqrt{20C_0c^3}}+\beta\ell(x)^{-1}\ . \tag{8.38}$$

Then for all x

$$f_1(x)\ell(x)\ \ge\ \beta\ . \tag{8.39}$$

Moreover,

$$R_1\cap Q_\beta^c\ \subset\ \Big\{x\mid \ell(x)\le C_1\frac{\beta}{\sqrt{-\mu}}\Big\}$$

and

$$R_2 \cap Q^c_\beta \;\subset\; \left\{x \;\middle|\; \ell(x) \geq C_2 \frac{\beta}{\sqrt{-\mu}}\right\} ,$$

where $C_1 = 6\sqrt{C_0(1+6c^3)+2}$ and $C_2 = \sqrt{C_0(1+4c^2)+2}$. Using this we derive

$$\frac{f_1(x)\ell(x)}{\beta} \;\leq\; \frac{f(x)\ell(x)}{\beta} + C_3$$

on $R_1 \cap Q^c_\beta$ and

$$\frac{\beta}{f_1(x)\ell(x)} \;\leq\; C_4 \frac{\beta}{\sqrt{-\mu}} \ell(x)^{-1}$$

on $R_2 \cap Q^c_\beta$, where C_3 and C_4 depend only on C_0 and c. These inequalities together with lemma 8.4 imply (8.36), provided that ψ is supported in Q^c_β. Since the case of ψ supported in $Q_{\frac{1}{2}\beta}$ is covered by theorem 8.1, eqn (8.36) is proven.

Now we apply theorems 8.1 and 8.4 to the operator K_β defined in (2.51). Recall that the potential $\phi(x) = \phi_\lambda(x,y)$ for this operator obeys (8.4) (see (2.9)) with $f(x)$ and $\ell(x)$ given in (2.7)–(2.8). The latter equations yield that these $f(x)$ and $\ell(x)$ obey (8.2)–(8.3).

Theorem 8.9. *Let K_β be the operator defined in (2.51). Let g, ψ and ρ be the same as in theorem 8.1 and let, besides, ψ be supported in $\{x \mid \ell(x) \geq r\}$ with $r \geq 0$. Then for any $\mu \leq 0$*

$$\begin{aligned} &\left|\mathrm{tr}\left(\psi g(K_\beta - \mu)\right) - \beta^{-d} \int\int \psi g(k-\mu)\right| \\ &\leq C\beta^{s+\rho-d} \max(r^{\frac{1}{2}}, \beta)^{-(3s+\rho-d)_+} + C\delta_s \left| \ln\left(\frac{\beta}{\sqrt{-\mu}}\right)\right| , \end{aligned} \tag{8.40}$$

where the constant is independent of β, of the λ_i's and of the y_i's and $\delta_s = 1$ if $s = 0$ and $= 0$ if $s \neq 0$.

Proof. We derive theorem 8.9 from theorem 8.7. Remembering that the potential of K_β obeys (8.4) with $f(x) = \ell(x)^{-\frac{1}{2}}\langle \ell(x)\rangle^{-\frac{3}{2}}$, we find that

$$\left\{x \;\middle|\; f(x)\ell(x) \geq \frac{1}{2}\beta\right\} \;\subset\; \{x \mid \beta^2 \leq \ell(x) \leq 2\beta^{-1}\} . \tag{8.41}$$

This and the fact that $\ell(x) = \min_j |x - y_j|$ yields that the first integral on the r.h.s. of (8.36) is bounded by the first term on the r.h.s. of (8.40).

To estimate the second integral on the r.h.s. of (8.36) we observe that

$$\{x \mid f(x)\ell(x) \le \beta\} \subset \{x \mid \ell(x) \le 4\beta^2\} \cup \{x \mid \ell(x) \ge \beta^{-1}\} . \tag{8.42}$$

The part of this integral over $\{x \mid \ell(x) \ge \beta^{-1}\}$ is bounded, clearly, by the second term on the r.h.s. of (8.40). The part over $\{x \mid \ell(x) \le 4\beta^2\}$ is, due to lemma 8.10 below, bounded by the first term on the r.h.s. of (8.40). Thus the second integral is bounded by the r.h.s. of (8.40). This together with the result of the previous paragraph implies (8.40).

Lemma 8.10. *Let $g(\lambda)$ obey $|g(\lambda)| \le -C\lambda_-^s$. Let ψ be smooth, supported in $\ell(x) \le r$ and obey $|\partial^\nu \psi(x)| \le C_\nu r^{-|\nu|}$. Then*

$$\|\psi(x) g(K_\beta)\|_1 \le C\Big(\frac{\max(r,\beta^2)}{\beta^2}\Big)^{3([d/2]+1)} \max(r,\beta^2)^{-s} , \tag{8.43}$$

provided either $r \le \beta^2$ and $0 \le s$ or $\beta^2 \le r \le \frac{1}{3}\min_{i\neq j} |y_i - y_j|$ and $s = 0$.

Proof. Due to the definition of $\ell(x)$ and the restriction $r \le \frac{1}{3} a$

$$\psi(x) = \sum \psi_i(x) , \tag{8.44}$$

where the functions ψ_i are smooth, supported in $|x - y_i| \le r$ and obey $|\partial^\nu \psi_i(x)| \le C_\nu r^{-|\nu|}$.

Next, rescaling $x \to y_i + rx$ maps K_β into $\frac{1}{r} K_{0,\beta}$, where

$$K_{0,\beta} = -\frac{\beta^2}{2r}\Delta - \phi_0(x) , \tag{8.45}$$

with $\phi_0(x) = r\big(\phi(y_i + rx) + \mu\big)$. Note that the r.h.s.'s of eqns (2.10) and (2.11) yields that $\phi(x) \le (\Sigma \lambda_j |x - y_j|^{-\frac{3}{2}})^{\frac{2}{3}} \le (\Sigma\lambda_j |x - y_j|^{-2})^{\frac{1}{2}}$. This together with the uncertainty principle $-\Delta \ge (4|x|^2)^{-1}$ implies that ϕ_0 obeys the Kato-type inequality

$$\|\phi_0 u\| \le \varepsilon\|\Delta u\| + \frac{C}{\varepsilon}\|u\| \tag{8.46}$$

for any $\varepsilon > 0$, $u \in D(\Delta)$ and with C independent of ε, β, M, y, λ and u. By the unitary invariance of the trace norm

$$\begin{aligned} &\|\psi_i(x) g_s(K_\beta)\|_1 \\ &= r^{-s} \|\psi_0(x) g_s(K_{0,\beta})\|_1 \;, \end{aligned} \tag{8.47}$$

where $g_s(\lambda) = \lambda_-^s$ and $\psi_0(x) = \psi_i(y_i + rx)$. Note that ψ_0 is smooth, supported in $|x| \leq 1$ and obeys $|\partial^\nu \psi(x)| \leq C_\nu$. We claim now that

$$\|\psi_0(x) g_s(K_{0,\beta})\|_1 \;\leq\; C\Big(\frac{r}{\beta^2}\Big)^{3([d/2]+1)} \;. \tag{8.48}$$

For $r = \beta^2$ (8.48) is, due to (8.46), a standard estimate (see e.g. [RSII]). For $s = 0$ and for general $r \geq \beta^2$ this follows from lemma 4.2.

Equations (8.47) and (8.48), the condition $|g(\lambda)| \leq -C g_s(\lambda)$ and the property of the trace norm yields that

$$\|\psi_i(x) g(K_\beta)\|_1 \;\leq\; C\Big(\frac{r}{\beta^2}\Big)^{3([d/2]+1)} r^{-s} \;.$$

This together with (8.44) yields (8.43).

9. Decoupling of Singularities

In the previous section we have proven rather accurate quasiclassical estimates outside of the singularities of the potential. In this section we show that inside a small neighbourhood of a singularity the spectral asymptotics of $\mathrm{tr}[\psi g(K_\beta)]$ can be computed by retaining in the potential $\phi(x)$ only the leading term near this singularity. In the next section we obtain asymptotics for the approximating Schrödinger operator near singularities.

Recall that we are considering the Schrödinger operator

$$K_\beta \;=\; -\frac{1}{2}\beta^2\Delta - \phi(x) \tag{9.1}$$

on ^{d}. In this section we assume that $\phi(x)$ is smooth outside the points $y_1, \ldots, y_M$ and obeys

$$|\partial^\nu \phi(x)| \;\le\; C_\nu \ell(x)^{-|\nu|-1}\langle \ell(x)\rangle^{-3} \;, \tag{9.2}$$

where $\ell(x) = \min_j |x - y_j|$. We assume, besides, that $\phi(x)$ can be written as

$$\phi(x) \;=\; \sum_{i=1}^{M} V_i(x) + \phi^{\mathrm{reg}}(x) \;, \tag{9.3}$$

where V_i and ϕ^{reg} are real functions, smooth outside y_i and $\{y_j\}$, respectively, and obeying

$$|\partial^\nu V_i(x)| \;\le\; C|x - y_i|^{-1-|\nu|} \tag{9.4}$$

and

$$|\partial^\nu \phi^{\mathrm{reg}}(x)| \;\le\; C\ell(x)^{-|\nu|}\langle \ell(x)\rangle^{-1} \;. \tag{9.5}$$

Consequently, near the singularities y_i we consider the Hamiltonians

$$K_{i,\beta} \;=\; -\frac{1}{2}\beta^2\Delta - V_i(x) \;.$$

The symbols of these operators are denoted by

$$k_i(x,\xi) \;=\; \frac{1}{2}|\xi|^2 - V_i(x) \;.$$

We assume in this section that $d \geq 2$. Let

$$g(\mu) \;=\; \mu_-$$

and recall that $a = \min\{|y_i - y_j|,\ i \neq j, 1\}$. In what follows $O(\cdots)$ stands for an estimate uniform in y and λ. The main result of this section is

Theorem 9.1. *Let K_β be defined in (9.1) with ϕ obeying (9.2)–(9.5), where M is bounded independently of β. Let $\beta^{\frac{2}{3}-\varepsilon} \leq r \leq \frac{1}{3}a$ for some $\varepsilon > 0$. Let $\psi \in C_0^\infty$ be supported in $\{x|\ell(x) \leq r\}$ and obey $\partial^\nu \psi = O(r^{-|\nu|})$. Then*

$$\begin{aligned} &\operatorname{tr}[\psi g(K_\beta) - \psi g(K_{i,\beta})] \\ &= \beta^{-d} \int\int \psi\big(g(k) - g(k_i)\big) \\ &\quad + O(\beta^{2-d} r^{\frac{d}{2}-2} + a^{-1}\beta^{1-d} r^{\frac{1}{2}(d-1)}) \end{aligned} \tag{9.6}$$

with the remainder estimate uniform in the y_j 's and in the λ_j 's.

Proof. We conduct the proof in two steps.

(a) On the first step we replace $\phi(x)$ by a potential $\widetilde{\phi}(x)$ s.t.

$$\widetilde{\phi}(x) \;=\; \begin{cases} V_i(x) & \text{for } |x - y_i| \leq 4r\ \forall i \\ \phi(x) & \text{for } \min|x - y_i| \geq 6r \end{cases} \tag{9.7}$$

and is obeying

$$|\partial^\nu \widetilde{\phi}(x)| \;\leq\; C\ell(x)^{-1-|\nu|}\langle \ell(x)\rangle^{-2} \tag{9.8}$$

and

$$\begin{aligned} &|\partial^\nu\big(\phi(x) - \widetilde{\phi}(x)\big)| \\ &\leq Ca^{-1}\ell(x)^{-|\nu|} \end{aligned} \tag{9.9}$$

with the constant C independent of a and r. $\widetilde{\phi}(x)$ can be constructed as

$$\widetilde{\phi}(x) \;=\; \sum_i V_i(x)\chi(x - y_i) + \phi(x)\big(1 - \sum_i \chi(x - y_i)\big)\ , \tag{9.10}$$

where $\chi(x)$ is supported in $|x| \leq 5r$ is $=1$ in $|x| \leq 4r$ and obeys $|\partial^\nu \chi(x)| \leq C_\nu r^{-\nu}$.

Denote

$$\widetilde{K}_\beta \;=\; -\frac{1}{2}\beta^2\Delta - \widetilde{\phi}(x) \tag{9.11}$$

and

$$\widetilde{k}(x,\xi) \;=\; \frac{1}{2}|\xi|^2 - \widetilde{\phi}(x) \;.$$

The main result at this step is the following

Lemma 9.2. *Let $\beta^2 \le r \le \frac{1}{3}a$ and let ψ be as in theorem 9.1. Then*

$$\begin{aligned} &\mathrm{tr}[\psi g(K_\beta) - \psi g(\widetilde{K}_\beta)] \\ &= \beta^{-3} \int\int \psi\big(g(k) - g(\widetilde{k})\big) \\ &\quad + O(\beta^{2-d} r^{\frac{d}{2}-2} + a^{-1}\beta^{1-d} r^{\frac{1}{2}(d-1)}) \;. \end{aligned} \tag{9.12}$$

Proof. Denote $K = K_\beta$ and $\widetilde{K} = \widetilde{K}_\beta$. Denote the l.h.s. of (9.13) by A and write

$$A \;=\; B + C \;, \tag{9.13}$$

where

$$B \;=\; -\mathrm{tr}\,\bar{\psi} g(K) + \mathrm{tr}\,\bar{\psi} g(\widetilde{K}) \;, \tag{9.14}$$

with $\bar{\psi} = 1 - \psi$, and

$$C \;=\; \mathrm{tr}\big(g(K) - g(\widetilde{K})\big) \;. \tag{9.15}$$

Applying theorem 8.9 with $\rho = 1$ and $s = 1$ to each term on the r.h.s. of (9.14), we obtain

$$\begin{aligned} B \;=\; &-\beta^{-d} \int\int \bar{\psi}\big(g(k) - g(\widetilde{k})\big) \\ &+ O(\beta^{2-d} r^{\frac{d}{2}-2}) \;. \end{aligned} \tag{9.16}$$

In order to estimate C we introduce the interpolating potential

$$\phi_t \;=\; \widetilde{\phi} + t(\phi - \widetilde{\phi}) \;.$$

Then C can be written as

$$C \;=\; \int_0^1 \mathrm{tr}\,\frac{\partial}{\partial t} g(K_t)\,dt \;, \tag{9.17}$$

where

$$K_t \;=\; -\frac{1}{2}\beta^2 \Delta - \phi_t(x) \;.$$

To calculate the r.h.s. we note that

$$g(K_t) \;=\; \int g(\lambda)\delta(K_t-\lambda)d\lambda \tag{9.18}$$

and

$$\delta(K_t-\lambda) \;=\; \frac{1}{2\pi}\,\mathrm{Im}(K_t-\lambda-i0)^{-1}\ .$$

Using the second resolvent equation, we find

$$\begin{aligned}&\frac{\partial}{\partial t}(K_t-z)^{-1}\\ =\;&-(K_t-z)^{-1}(\phi-\widetilde{\phi})(K_t-z)^{-1}\ .\end{aligned}$$

By the cyclic property of the trace

$$\begin{aligned}&\mathrm{tr}[(K_t-z)^{-1}(\phi-\widetilde{\phi})(K_t-z)^{-1}]\\ =\;&\mathrm{tr}[(\phi-\widetilde{\phi})(K_t-z)^{-2}]\ .\end{aligned}$$

The last three relations yield

$$\begin{aligned}&\mathrm{tr}\,\frac{\partial}{\partial t}\,\delta(K_t-\lambda)\\ =\;&-\frac{\partial}{\partial\lambda}\,\mathrm{tr}[(\phi-\widetilde{\phi})\delta(K_t-\lambda)]\ .\end{aligned}$$

Integrating this equation against $g(\lambda)$ and then integrating the r.h.s. by parts and using (9.18) for the l.h.s., we find

$$\mathrm{tr}\,\frac{\partial}{\partial t}g(K_t) \;=\; -\mathrm{tr}[(\phi-\widetilde{\phi})g'(K_t)]\ . \tag{9.19}$$

Here $g'(\lambda) = \frac{\partial g(\lambda)}{\partial\lambda}$, the indicator function of $(-\infty,0]$. This together with eqn (9.14) yields

$$C \;=\; -\int_0^1 \mathrm{tr}[(\phi-\widetilde{\phi})g'(K_t)]dt\ . \tag{9.20}$$

Pick now r_0 obeying

$$\beta^2 \;=\; r_0 \;<\; r\ . \tag{9.21}$$

Using that $\phi - \widetilde{\phi}$ is supported in $B(0,6r)$ and obeys estimate (9.8), applying (8.5) with $f(x) = \ell(x)^{-\frac{1}{2}}$, $s = 0$ and $\rho = 1$ ($d \geq 2$) in $\Omega = \{x | r_0 \leq \ell(x) \leq 6r\}$ and rough estimate (8.43) in $\{x | \ell(x) \leq 2r_0\}$ to the r.h.s. of (9.20), we obtain

$$|C - \mathrm{Weyl}| \;\leq\; \mathrm{const}\, I \;,$$

where

$$\begin{aligned} \mathrm{Weyl} \;&=\; -\beta^{-d} \int\!\!\int \int_0^1 (\phi - \widetilde{\phi}) g'(k_t) dt \\ &=\; \beta^{-d} \int\!\!\int [g(k) - g(\widetilde{k})] \end{aligned}$$

and

$$\begin{aligned} I \;&= a^{-1}\beta^{1-d} \int_{r_0}^{6r} t^{\frac{d}{2}-\frac{1}{2}} \frac{dt}{t} \\ &\quad + a^{-1}\beta^{-d} \int_0^{2r_0} t^{\frac{d}{2}} \frac{dt}{t} \;. \end{aligned}$$

Since $r_0 \leq r$ and $d > 1$, the first integral is bounded by $\mathrm{const}\, r^{\frac{1}{2}(d-1)}$. The second integral is bounded by $\mathrm{const}\, r_0^{\frac{d}{2}} = \mathrm{const}\, \beta^d$. Hence for $r \geq \beta^2$

$$\begin{aligned} C \;&= \beta^{-d} \int\!\!\int [g(k) - g(\widetilde{k})] \\ &\quad + O(a^{-1}\beta^{1-d} r^{\frac{1}{2}(d-1)}) \;. \end{aligned} \tag{9.22}$$

Combining (9.13), (9.16) and (9.22), we arrive at (9.12).

(b) Now we pass from $\widetilde{K}_\beta$ to $K_{i,\beta}$. The main result at this step is

Lemma 9.3. *Let $\varphi(\lambda)$ be a smooth function on obeying $|\partial^n \varphi(\lambda)| \leq C_n \langle\lambda\rangle^{n+m}$ for some m. Let $\psi \in C_0^\infty\big(B(y_i, r)\big)$ and obey $|\partial^\nu \psi(x)| \leq C_\nu r^{-|\nu|}$. Let $r \geq \beta^2$. Then for any $A \geq \left[\frac{d}{2}\right] + 2$*

$$\begin{aligned} &\|\psi(x)\big(\varphi(\widetilde{K}_\beta) - \varphi(K_{i,\beta})\big)\|_1 \\ &\leq C\|\varphi\|_A \Big(\frac{\beta}{r^{3/2}}\Big)^A \Big(\frac{\beta}{r}\Big)^{-3d-12} \;, \end{aligned} \tag{9.23}$$

where $\|\varphi\|_A = \sup_\lambda(\langle\lambda\rangle^{A+m} |\partial_\lambda^{A+m} \varphi(\lambda)|)$ and C is independent of β and r.

Proof. Rescale the problem as $x \to y_i + rx$. Then

$$\widetilde{K}_\beta \;\to\; H_\beta \qquad \text{and} \qquad K_{i,\beta} \;\to\; H_{0,\beta} \;, \tag{9.24}$$

where

$$H_\beta \;=\; -\frac{1}{2}\Big(\frac{\beta}{r}\Big)^2\Delta - \widetilde{\phi}(y_i+rx)\ , \tag{9.25}$$

and

$$H_{0,\beta} \;=\; -\frac{1}{2}\Big(\frac{\beta}{r}\Big)\Delta - V_i(y_i+rx)\ . \tag{9.26}$$

Observe that $\widetilde{\phi}(y_i+rx) = V_i(y_i+rx)$ on $B(0,2)$ and that $\sup\limits_{B(0,2)\setminus B(0,1)} \widetilde{\phi}(y_i+rx) \le Cr^{-1}$. Furthermore, we have

$$\begin{aligned} &\|\psi(x)\big(\varphi(\widetilde{K}_\beta) - \varphi(K_{i,\beta})\big)\|_1 \\ &\le C\|\psi_1(x)\big(\varphi(H_\beta) - \varphi(H_{0,\beta})\big)\|_1 \end{aligned} \tag{9.27}$$

where $\psi_1(x) = \psi\Big(\frac{x-y_i}{r}\Big) \in C_0^\infty\big(B(0,1)\big)$. $\psi_1(x)$ obeys $|\partial^\nu\psi_1(x)| \le C_\nu$. Applying theorem 4.6 with $\alpha = \frac{\beta}{r}$, and $L = r^{-\frac{1}{2}}$, to the r.h.s., we arrive at (9.23).

Lemma 9.4. *Let $g(\mu) = \mu_-$ and let $\psi \in C_0^\infty\big(B(y_i,r)\big)$ and satisfy $|\partial^\nu\psi(x)| \le C_\nu \ell(x)^{-|\nu|}$. Let $\frac{1}{3}a > r \ge \beta^{\frac{2}{3}-\varepsilon}$ for some $\varepsilon > 0$. Then*

$$\begin{aligned} &\|\psi g(\widetilde{K}_\beta)\psi - \psi g(K_{i,\beta})\psi\|_1 \\ &\le C\beta^{1-d} r^{\frac{d-1}{2}}\ . \end{aligned} \tag{9.28}$$

Proof. As is the proof of lemma 9.2 we set $K = \widetilde{K}_\beta$ and $K_0 = K_{i,\beta}$. Pick f_1 and f_2, obeying

$$f_1(\mu) + f_2(\mu) \;=\; g(\mu)\ ,$$

$$\operatorname{supp} f_1 \;\subset\; [-3,0]\ ,$$

and

$$\operatorname{supp} f_2 \;\subset\; (-\infty,-2)\ ,$$

besides f_2 is taken to be smooth. We have

$$\operatorname{tr}\big(\psi g(K)\psi - \psi g(K_0)\psi\big) \;=\; \sum_{i=1}^{2} A_i\ , \tag{9.29}$$

where

$$A_i \;=\; \operatorname{tr}\big(\psi f_i(K)\psi - \psi f_i(K_0)\psi\big)\ .$$

Consider A_1. Decompose ψ in a smooth way as

$$\psi \ = \ \psi_1 + \psi_2 \ ,$$

where ψ_1 is supported in $B(y_i, 2r_0)$ and ψ_2, in $B(y_i, r)\backslash B(y_i, r_0)$ with $r_0 = \beta^2$. Applying rough estimate (8.43) in which ψ, g and r are replaced by ψ_1, f_1 and r_0, respectively, we obtain

$$\begin{aligned} 0 \ &\leq \ \operatorname{tr} \psi_1 f_1(K) \psi_1 \\ &\leq \ C \left(\frac{r_0}{\beta^2} \right)^{3([d/2]+1)} \end{aligned}$$

and similarly for K_0. Hence

$$\begin{aligned} &\operatorname{tr} \psi_1 f_1(K) \psi_1 - \operatorname{tr} \psi_1 f_1(K_0) \psi_1 \\ &\leq \ C \Big(\frac{r_0}{\beta^2} \Big)^{3([d/2]+1)} \ . \end{aligned} \tag{9.30}$$

Next, we apply to $\operatorname{tr}[\psi_2^2 f_1(K)]$ and $\operatorname{tr}[\psi_2^2 f_1(K_0)]$ eqn (8.5) with $s = 0$, with $d \geq 2$ and therefore $\rho = 1$, with $\Omega = \{ r_0 \leq |x - y_i| \leq r \}$ and with $\ell(x) = \min |x - y_j|$ and $f(x) = \ell(x)^{-\frac{1}{2}}$. Taking into account that

$$\psi_2 \big(f_1(k) - f_1(k_0) \big) \ = \ 0 \ ,$$

where $k = k^{(i)}$ and $k_0 = k_i$, we obtain

$$\begin{aligned} &|\operatorname{tr} \big(\psi_2^2 f_1(K) - \psi_2^2 f_1(K_0) \big)| \\ &\leq C \beta^{1-d} \int_{r_0}^{r} t^{\frac{d-1}{2}} \frac{dt}{t} \\ &\leq C \beta^{1-d} r^{\frac{d-1}{2}} \ . \end{aligned} \tag{9.31}$$

Combining (9.30) and (9.31) and remembering that $r_0 = \beta^2$ and $r \geq \beta^2$, we find

$$|A_1| \ \leq \ C \beta^{1-d} r^{\frac{d-1}{2}} \ . \tag{9.32}$$

Next, applying lemma 9.3 to the r.h.s. of

$$|A_2| \ \leq \ \| \psi f_2(K) \psi - \psi f_2(K_0) \psi \|_1 \ ,$$

we obtain that for any $B \geq 0$

$$|A_2| \;\leq\; C\beta^B \; .$$

This together with (9.29) and (9.32) yields (9.28).

Lemmas 9.2 and 9.4 imply theorem 9.1.

10. Coulomb Problem

In this section we compute some spectral characteristics of the Coulomb problem. We use the following notation

$$K_{\lambda,\beta} \;=\; -\frac{1}{2}\beta^2\Delta - \frac{\lambda}{|x|} + \lambda$$

with $\lambda > 0$ on $L^2(^3)$ and

$$k_\lambda \;=\; \frac{1}{2}|\xi|^2 - \frac{\lambda}{|x|} + \lambda \; . \tag{10.1}$$

Let ψ be a smooth function on $[0,\infty)$ with the properties

$$\psi(t) \;=\; \begin{matrix} 1 & \text{for } t \leq 1 \\ 0 & \text{for } t \geq 2 \end{matrix} \; .$$

ψ_r will stand either for $\psi(|x|/r)$ or for $\psi(t/r)$ or for the multiplication operators related to the latter functions. Let

$$g(\mu) \;=\; \mu_- \;\equiv\; \begin{cases} \mu & \text{if } \mu \leq 0 \\ 0 & \text{if } \mu > 0. \end{cases}$$

The main result of this section is

Theorem 10.1. *Let* $\beta^2 \leq r \leq 1$ *and let* $\psi \in C_0^\infty\big(B(0,2r)\big)$ *and obey* $|\partial^\nu\psi| \leq C_\nu r^{-|\nu|}$ *. Then, with the remainder uniform in* λ *,*

$$\begin{aligned} \operatorname{tr}\big(\psi g(K_{\lambda,\beta})\big) \;&= \beta^{-3}\int\int \psi g(k_\lambda) \\ &\quad + \frac{1}{8}\beta^{-2}\lambda^2 + O(\beta^{-1}r^{-\frac{1}{2}}\lambda^{\frac{1}{2}}) \end{aligned} \tag{10.2}$$

with $O(\beta^{-1}r^{-\frac{1}{2}})$ *uniform in* β *,* r *and* λ *.*

Proof. To begin with we rewrite $K_{\lambda,\beta}$ as

$$K_{\lambda,\beta} \;=\; \lambda K_\gamma \qquad \text{with} \quad \gamma = \frac{\beta}{\sqrt{\lambda}} \tag{10.3}$$

and with

$$K_\gamma \;=\; -\frac{1}{2}\gamma^2\Delta - \frac{1}{|x|} + 1 \; . \tag{10.4}$$

Let $\overline{\psi} = 1 - \psi$. Applying theorem 8.1 with $\ell(x) = |x|$ and $f(x) = |x|^{-\frac{1}{2}}$, we obtain

$$\operatorname{tr}\big(\overline{\psi} g(K_\gamma)\big) \;=\; \gamma^{-3} \int\!\!\int \overline{\psi} g(k) + O(\gamma^{-1} r^{-\frac{1}{2}}) \ , \tag{10.5}$$

where $k = \frac{1}{2}|\xi|^2 - \frac{1}{|x|} + 1$, provided $r \geq \beta^2$. Next we compute $\operatorname{tr} g(K_\gamma)$. The eigenvalues of K_γ are

$$E_n = -\frac{1}{2\alpha^2 n^2} + 1 \tag{10.6}$$

with the multiplicities n^2 . Hence

$$\operatorname{tr} g(K_\gamma) \;=\; \sum_{n=1}^{m} \Big(1 - \frac{1}{2\alpha^2 n^2}\Big) n^2 \ , \tag{10.7}$$

where $m = \left[\frac{1}{\sqrt{2}\gamma}\right]$. Computing the sum on the r.h.s., we find

$$\operatorname{tr} g(K_\gamma) \;=\; \frac{1}{3} m(m+1)(m+\frac{1}{2}) - \frac{1}{2}\alpha^{-2} m \ . \tag{10.8}$$

Representing m as $m = \frac{1}{\sqrt{2}\gamma} - t$ for some $t \in [0,1]$, we see that the r.h.s. can be simplified as

$$\operatorname{tr} g(K_\gamma) \;=\; -\frac{1}{3\sqrt{2}\gamma^3} + \frac{1}{4\gamma^2} + O(\gamma^{-1}) \ . \tag{10.9}$$

On the other hand we can compute explicitly

$$\int\!\!\int g(k) \;=\; -\frac{1}{3\sqrt{2}} \ . \tag{10.10}$$

Combining the last two relations yields

$$\begin{aligned} \operatorname{tr} g(K_\gamma) \;&= \gamma^{-3} \int\!\!\int g(k) \\ &\quad + \frac{1}{4}\gamma^{-2} + O(\gamma^{-1}) \ . \end{aligned} \tag{10.11}$$

Equations (10.5) and (10.11) and the observation that $\operatorname{tr}[\psi g(K_{\lambda,\beta})] = \lambda \operatorname{tr} \psi g(K_\gamma)$ with $\gamma = \frac{\beta}{\sqrt{\lambda}}$ yields (10.2).

11. Estimates of Schwartz Kernels

In this section we study the restriction $e(x,x,\lambda,H_\alpha)$ of the Schwartz kernel of the operator $E(\lambda,H_\alpha)$ to the diagonal. Recall

$$e_0(x,\lambda,H_\alpha) \;=\; \alpha^{-d}\int_{h(x,\xi)\le\lambda} d\xi \;,$$

the Weyl expression for $e(x,x,\lambda,H_\alpha)$. We begin with the following result (cf. Hörm 1968).

Theorem 11.1. *Let H_α be defined as in the beginning of section 4. Let $\alpha\le 1$. For $x\in B(0,1)$*

$$\begin{aligned}&|e(x,x,\lambda,H_\alpha)-e_0(x,\lambda,H_\alpha)|\\ &\le\; C\alpha^{1-d}(|W(x)+\lambda|+\alpha^{\frac{2}{3}})^{\frac{d-3}{2}}\end{aligned} \tag{11.1}$$

where C is independent of α. In particular, for $d\ge 3$

$$|e(x,x,\lambda,H_\alpha)-e_0(x,\lambda,H_\alpha)| \;\le\; C\alpha^{1-d} \tag{11.2}$$

and for $d=1,2$ the r.h.s. is at most $O(\alpha^{-\frac{2d}{3}})$.

Proof. First we assume that x belongs to a closed subset of

$$\{x\in\overline{B(0,1)}|W(x)\ne-\lambda\} \tag{11.3}$$

and prove (11.2) with this additional restriction. Then using this result and the multiscale analysis of section 8, we remove this condition.

If $W(x)<-\lambda$, then $e_0(x,\lambda,H_\alpha)=0$ and

$$e(x,x,\lambda,H_\alpha) \;=\; O(\alpha^M)$$

for any M by an estimate similar to (4.28), reflecting the fact that x is in the classically forbidden region. Thus it suffices to consider the case $W(x)\ge-\lambda$.

As before, let χ be a smooth function whose α-Fourier transform $\widehat{\chi}$ is smooth and supported in a sufficiently small neighbourhood of $t=0$ and let χ_1 be defined by

$$\chi(\lambda) \;=\; \frac{1}{\alpha}\chi_1\left(\frac{\lambda}{\alpha}\right) \;.$$

First we study $\chi * dE$ and then, using the Tauberian technique, extract from this study the information about E.

To estimate $\chi * dE$ we write it as

$$\chi * dE(\lambda, H_\alpha) \;=\; \frac{1}{2\pi\alpha}\int \widehat{\chi}(t)e^{i\lambda t/\alpha}U(t)dt \;.$$

Using the decomposition

$$U(t) \;=\; F(t) + G(t) \;,$$

where F is the Fourier integral operator introduced in section 4 and G is defined by this equation, we split (11.2) as

$$\chi * dE \;=\; \frac{1}{\alpha}F_\chi + \frac{1}{\alpha}G_\chi \;,$$

where

$$F_\chi(\lambda) \;=\; \int e^{i\lambda t/\alpha}\widehat{\chi}(t)F(t)dt \tag{11.4}$$

and

$$G_\chi(\lambda) \;=\; \int e^{i\lambda t/\alpha}\widehat{\chi}(t)G(t)dt \;. \tag{11.5}$$

Denote the restriction of the kernel of $F_\chi(\lambda)$ to the diagonal by $f(\lambda, x)$.

Lemma 11.2. *Under the conditions of theorem 11.1 and the restriction* $W(x) > -\lambda$ *on* $\overline{B(0,1)}$ *we have*

$$f(x,\lambda) \;=\; e_0(x,\lambda,H_\alpha) + O(\alpha^{1-d}) \tag{11.6}$$

with the uniformly bounded error term.

Proof. Substituting into (11.4) expression (4.3) for $F(t)$, taking the kernel of the resulting operator and restricting it to the diagonal, we derive

$$f(x,\lambda) \;=\; \alpha^{-d}\int\int e^{i\phi/\alpha}bd\xi dt \;, \tag{11.7}$$

where $b = \widehat{\chi}a$ and

$$\phi \;=\; S - x \cdot \xi + \lambda t \; .$$

Due to lemma A.2 of the Appendix

$$\begin{aligned} \partial_t \phi &= \lambda - h - \xi \cdot \nabla W t + O(t^2 \langle \xi \rangle) \\ \partial_\xi \phi &= -\xi t + O(t^2 \langle \xi \rangle) \; . \end{aligned}$$

Of course, similarly to the previous case,

$$\{(t,\xi) | t = 0,\; h(x,\xi) \;=\; \lambda\} \tag{11.8}$$

is the family of critical manifolds of ϕ labeled by x. There are no other critical points due to the condition that $W(x) \neq -\lambda$. On (11.8)

$$\begin{aligned} \mathrm{Hess}_{(t,\xi)} \phi &= |\xi| \\ &= \sqrt{2\big(W(x) + \lambda\big)} \; , \end{aligned}$$

which is positive since $W(x) > -\lambda$. Hence stationary phase technique can be applied and a derivation similar to the proof of theorem 5.2 produces the desired result.

Lemma 11.3. *The kernel $g(\lambda, x, z)$ of $G_\chi(\lambda)$ obeys the estimate*

$$|g(\lambda, x, z)| \;\leq\; C\alpha^{N-12-3d} \; , \tag{11.9}$$

where N is the same as in (5.6).

Proof. To simplify the exposition we restrict ourselves to the case $d \leq 3$. Let $\psi \in C_0^\infty\big(B(0, \frac{3}{2})\big)$ and $\psi = 1$ on $B(0,1)$. We write

$$\psi G_\chi \psi \;=\; (-\Delta + 1)^{-1} A (-\Delta + 1)^{-1} \; ,$$

where

$$A \;=\; (-\Delta + 1) \psi G_\chi \psi (-\Delta + 1) \; .$$

Since $d \leq 3$, the kernel $K(x-z)$ of $(-\Delta+1)^{-1}$ obeys

$$\int |K(x)|^2 dx \; < \; \infty \; .$$

Since for $x, z \in B(0,1)$

$$\begin{aligned} & g(\lambda, x, z) \\ = & \langle K(x-\cdot), AK(\cdot - z)\rangle \; , \end{aligned}$$

we have

$$\begin{aligned} & |g(\lambda, x, z)| \\ \leq & \|A\| \, \|K\|^2 \; . \end{aligned}$$

It is shown similarly to lemma 5.2 (see especially equations (5.17)–(5.18)) that

$$\|A\| \; \leq \; C\alpha^{N-12-d} \; ,$$

where N is the same as in (4.6). The last two inequalities yield

$$|g(\lambda, x, z)| \; \leq \; C\alpha^{N-12-d} \; .$$

In the general case we replace $(-\Delta+1)^{-1}$ by $(-\Delta+1)^{-[\frac{d}{2}]-1}$ which worsens the estimate correspondingly.

Lemmas 11.2 and 11.3 imply that $\chi * de - \chi * de_0 = O(\alpha^{1-d})$, provided (11.3) holds. This and the Tauberian technique (see section 7) yields that $e - e_0 = O(\alpha^{1-d})$ under condition (11.3). Using now multiscale analysis of section 8, we remove the restriction $W(x) \neq -\lambda$. Since the previous result is applicable to the region

$$\{x| \, |W(x)+\lambda| \geq 1\} \; ,$$

it suffices to consider x from

$$\{x| \, |W(x)+\lambda| \leq 1\} \; .$$

On this domain we introduce the coordinate scale

$$\ell(x) \; = \; M_1^{-1}|W(x)+\lambda| + \alpha^{\frac{2}{3}} \; , \tag{11.10}$$

where $M_1 = 2 \sup\limits_{B(0,2)} |\nabla W(x)|$. A simple analysis, similar to one already done in the proof of theorem 8.3, shows that if we introduce the energy scale as

$$\begin{aligned} f(x) &= M_1^{\frac{1}{2}} \ell(x)^{\frac{1}{2}} \\ &\sim |W(x) + \lambda|^{\frac{1}{2}} + \alpha^{\frac{1}{3}} \end{aligned} \tag{11.11}$$

then the shifted potential $\phi(x) = W(x) + \lambda$ obeys (8.2)–(8.4). Moreover, the scales satisfy $f\ell \geq \beta$.

As in the proof of theorem 8.3 we have to check that the rescaled potential

$$\widetilde{W}(x) = f(x)^{-2}\Big(W\big(y + \ell(y)x\big) + \lambda\Big)$$

obeys the initial restriction $\widetilde{W}(x) \neq 0$. Indeed, we have

$$\begin{aligned} |\widetilde{W}(x)| &= \frac{\ell\big(y + \ell(y)x\big)}{M_1 \ell(y)} \\ &\geq 1 - \frac{1}{M_1} \sup_{B(0,1)} |\nabla W(x)| \\ &\geq \frac{1}{2} \end{aligned}$$

on $B(0,1)$. Thus the previous result is applicable to the rescaled (in coordinate and energy) Hamiltonian

$$\widetilde{H}_\alpha = -\left(\frac{\alpha}{f\ell}\right)^2 \Delta - \widetilde{W}(x) \tag{11.12}$$

and the unit ball $B(0,1)$. Recall that this Hamiltonian is related to the original one by

$$f^{-2} U(\ell) H_\alpha U(\ell)^{-1} = \widetilde{H}_\alpha , \tag{11.13}$$

where $U(\ell)$ is the unitary family realizing the scaling $x \mapsto y + \ell x$. This relation implies

$$\begin{aligned} &\langle x | E(\lambda, \widetilde{H}_\alpha) | z \rangle \\ &= \langle x | U(\ell) E(\lambda f^2, H_\alpha) U(\ell)^{-1} | z \rangle \\ &= \ell^d \langle y + \ell x | E(\lambda f^2, H_\alpha) | y + \ell z \rangle , \end{aligned} \tag{11.14}$$

where we have used the notation $\langle x|A|z\rangle$ for the Schwartz kernel of an operator A. (Eqn (11.14) reflects the fact that $\langle x|A|z\rangle$ is a function in x and density in z.) Using this relation we derive as in theorem 8.1

$$\begin{aligned}&|e(x,x,\lambda,H_\alpha)-e_0(x,\lambda,H_\alpha)|\\ &\le C\alpha^{1-d}\big(\ell(x)f(x)\big)^{d-1}\ell(x)^{-d}\\ &= C\alpha^{1-d}\ell(x)^{-1}f(x)^{d-1}\ .\end{aligned}$$

Remembering (11.10) and (11.11), we deduce from this (11.1).

Now we return to the operator

$$K_\beta \;=\; -\frac{1}{2}\beta^2\Delta_x-\phi(x)\ . \tag{11.15}$$

In this section we will also use the following stronger version of Kato inequality (8.1):

$$\|\phi u\| \;\le\; \varepsilon\|\Delta u\|+\frac{C}{\varepsilon}\|u\| \tag{11.16}$$

for any $\varepsilon>0$, for any $u\in D(\Delta)$ and for some C independent of ε and of u.

Theorem 11.4. *Assume K_β defined in (11.15) obeys conditions (11.16) and (8.2)–(8.4) and let $d\ge 3$. Then for all x and for all $\mu\le 0$*

$$\begin{aligned}&|e(x,x,\mu,K_\beta)-e_0(x,\mu,K_\beta)|\\ &\le C\Big[\min\Big(\frac{\beta}{f(x)\ell(x)},1\Big)\Big]^{1-d}\big[\max\big(\ell(x),\beta^2\big)\big]^{-d}\ .\end{aligned} \tag{11.17}$$

Proof. In the region $\{x\mid f(x)\ell(x)\ge\beta\}$ one uses theorem 11.1 as a starting point and then follows the proof of theorem 8.1. The connection between the Schwartz kernels of spectral projections for the original and rescaled Schrödinger operators is given in

$$e(x,z,\mu,K_\beta) \;=\; \ell^{-d}e\Big(\frac{x-y}{\ell},\frac{x-y}{\ell},f^{-2}\mu,H_\alpha\Big)\ , \tag{11.18}$$

where $H_\alpha=f^{-2}U(\ell)K_\beta U(\ell)^{-1}$ with $\alpha=\frac{\beta}{f\ell}$ and $U(\ell):\ f(x)\to\ell^{-\frac{d}{2}}f\Big(\frac{x-y}{\ell}\Big)$. We will not repeat the arguments here referring the interested reader to the proof of theorem 8.1.

Now we consider the region $\{x \mid f(x)\ell(x) \le 2\beta\}$. First we notice that the explicit formula

$$e_0(x,\mu,K_\beta) \;=\; C_d\beta^{-d}\big(\phi(x)+\mu\big)_+^{\frac{d}{2}}\,, \tag{11.19}$$

where C_d is the volume of the unit d-sphere S^d times $\frac{1}{d}$, implies that for $\mu \le 0$

$$\begin{aligned} 0 \;\le\; e_0(x,\mu,K_\beta) \;&\le\; C\beta^{-d}\phi(x)_+^{\frac{d}{2}} \\ \le\; C\beta^{-d}f(x)^d \;&=\; C\Big(\frac{\beta}{f(x)\ell(x)}\Big)^{-d}\ell(x)^{-d}\,. \end{aligned} \tag{11.20}$$

Thus in $\{x \,\big|\, f(x)\ell(x) \le \beta\}$, the function $e_0(x,\mu,K_\beta)$ is bounded by the r.h.s. of (11.17).

Lemmas 11.5 and 11.6 below yield for $\mu \le 0$ and for x in $\{x \mid f(x)\ell(x) \le 2\beta\}$

$$e(x,x,\mu,K_\beta)| \;\le\; C\big[\max\big(\beta^2,\ell(x)\big)\big]^{-d} \tag{11.21}$$

with C independent of μ and of β. Therefore $|e(x,x,\mu,K_\beta)|$ is bounded by the r.h.s. of eqn (11.17) in the region $\{x \,\big|\, f(x)\ell(x) \le 2\beta\}$ and for $\mu \le 0$. This together with the conclusions of the previous two paragraphs yields (11.17).

Lemma 11.5. *Let K_β be defined by (11.15) with ϕ obeying (8.1)–(8.4). Then*

$$|e(x,x,\mu,K_\beta)| \;\le\; C\ell(x)^{-d}\max\Big(\frac{f(x)\ell(x)}{\beta},1\Big)^{2(d+2)} \tag{11.22}$$

for $\mu \le 0$ for all x and uniformly in β and in μ.

Proof. We begin with a general remark. For a self-adjoint operator B on $L^2(^d)$ we introduce

$$A(B,\mu,\psi_i) \;=\; (-\Delta+i)^{[\frac{d}{2}]+1}\psi_1 E(\mu,B)\psi_2(-\Delta+1)^{[\frac{d}{2}]+1}\,. \tag{11.23}$$

We have as in the proof of lemma 11.3 that

$$|e(z,z',\mu,B)| \;\le\; C\|A(\beta,\mu,\psi_i)\|\,, \tag{11.24}$$

provided $\psi_1(z)=1$ and $\psi_2(z')=1$. Here C depends only on the dimension d. Now we proceed to specific estimates.

We rescale K_β using the transformation $x \to y + \ell x$ which maps it unitarily into $\frac{\beta^2}{\ell^2} H$, where $H = -\frac{1}{2}\Delta_x - \phi_0(x)$ with $\phi_0(x) = \beta^{-2}\ell^2\phi(y+\ell x)$. Using the properties of $f(x)$, we obtain

$$\begin{aligned} |\partial^\nu \phi_0(x)| \ &\leq \ C_\nu \Big(\frac{f(y+\ell x)\ell}{\beta}\Big)^2 \\ &\leq \ C_\nu \Big(\frac{f\ell}{\beta}\Big)^2 \ \leq \ C_\nu \quad \text{on } B(0,1)\ , \end{aligned} \tag{11.25}$$

where $f = f(y)$. Pick up $\mu \leq 0$, $\psi_1 \in C_0^\infty\big(B(z,1)\big)$ and $\psi_2 \in C_0^\infty\big(B(z',1)\big)$. Using either lemma 4.2 or lemma 4.5, we obtain that

$$\begin{aligned} &\|A(H,\mu,\psi_i)\| \\ &\leq C \ \max\Big(\frac{f\ell}{\beta},\ 1\Big)^{2(d+2)} A_1(H,\mu,\phi_i) \end{aligned}$$

where

$$A_1(H,\mu,\varphi_1) \ = \ \|(H+i)^{[\frac{d}{2}]+1}\varphi_1 E(\mu,H)\varphi_2(H-i)^{[\frac{d}{2}]+1}\|\ ,$$

$\varphi_1 \in C_0^\infty\big(B(z,2)\big)$ and $=1$ on $B(z,1)$ and $\varphi_2 \in C_0^\infty\big(B(z',2)\big)$ and and $=1$ on $B(z',1)$ and commuting $(H\pm i)^{[\frac{d}{2}]+1}$ one by one through φ_1/φ_2, and using estimates similar to those employed in section 4, we obtain

$$\|A_1(H,\mu,\varphi_i)\| \leq C\sum_{k=0}^{d+2}\|\chi_1 f_k(H)\chi_2\|\ ,$$

where $\chi_1 \in C_0^\infty\big(B(z,3)\big)$ and $=1$ on $B(z,2)$, $\chi_2 \in C_0^\infty\big(B(z',3)\big)$ and $=1$ on $B(z',2)$ and $f_k(\lambda) = (|\lambda|^2+1)^{\frac{k}{2}}E(\mu,\lambda)$. By a special case of theorem 4.10, $\|\chi_1 f_k(H)\chi_2\| \leq C$, uniformly in β and $\mu \leq 0$. This together with the last two inequalities yields

$$\|A(H,\mu,\psi_i)\| \ \leq \ C \ \max\Big(\frac{f\ell}{\beta},1\Big)^{2(d+2)}$$

uniformly in β and $\mu \leq 0$. Due to (11.24) this yields

$$|e(z,z',\mu,H)| \ \leq \ C \ \max\Big(\frac{f\ell}{\beta},1\Big)^{2(d+2)} \tag{11.26}$$

uniformly in β and $\mu \leq 0$. Remembering now (11.18) and taking there $x = z = y$, we arrive at (11.22).

Lemma 11.6. *Assume that K_β is defined by (11.15) with $\phi(x)$ obeying (11.16). Then for any x and $\mu \le 0$*

$$|e(x,x,\mu,K_\beta)| \;\le\; C\beta^{-2d} \tag{11.27}$$

with C independent of β and μ.

Proof. For some fixed y, the scaling $x \to y+\beta^2 x$ maps K_β into $\beta^{-2}H$, where $H = -\frac{1}{2}\Delta - \phi_0(x)$ with $\phi_0(x) = \beta^2\phi(y+\beta^2 x)$. It is readily checked that also the new potential $\phi_0(x)$ satisfies inequality (11.16). By lemma 4.2

$$\|A(H,\mu,\psi_i)\| \;\le\; C$$

uniformly in β and in μ provided $\psi_i \in C_0^\infty\big(B(0,1)\big)$ and $\mu \le 0$. This, in turn, yields, due to (11.24), that

$$|e(x,z,\mu,H)| \;\le\; C$$

for $x,z \in B(0,1)$ and $\mu \le 0$. On the other hand the Schwarz kernels for $E(\mu,K_\beta)$ and $E(\mu,H)$ are related as

$$e(x,z,\mu,K_\beta) \;=\; \beta^{-2d} e\Big(\frac{x-y}{\beta^2}, \frac{z-y}{\beta^2}, \beta^2\mu, H\Big)\ .$$

Taking here $x=z=y$ and then using the previous inequality one obtains (11.27).

Let $\ell(x) = \min|x-y_j|$ for some $y_1, \ldots, y_M$. Then performing integrations carefully and using that

$$\int_{\ell(x)\le 1} \ell(x)^{-\mu} dx + \int_{\ell(x)\ge 1} \ell(x)^{-\nu} dx \;\le\; CM\ ,$$

provided $0<\mu<1<\nu$, we derive from theorem 11.4 the following

Corollary 11.7. *Assume K_β, defined in (11.15), obeys (11.16) and (8.2)–(8.4) with $\ell(x)$ replaced by $\ell_1(x) = L\ell(x)$ for some $L>0$ and with $f(x) = \ell(x)^{-\frac{1}{2}}\langle\ell(x)\rangle^{-\frac{3}{2}}$, where $\ell(x) = \min|x-y_j|$ for some $y_1,\ldots,y_M$. Let $d=3$. Then for any $\mu \le 0$ and for any $p \in \Big(1,\frac{3}{2}\Big)$*

$$\Big(\int |e(x,x,\mu,K_\beta) - e_0(x,\mu,K_\beta)|^p dx\Big)^{\frac{1}{p}}$$
$$\le CL^{d-1}M^{\frac{1}{p}}\beta^{1-d}$$

with C independent of β, of μ, of M, of the y_j 's and, in general, of $\phi(x)$.

Remark 11.8. The condition $d \geq 3$ (or the extra term $|W(x)+\lambda|^{(d-3)/2}$ on the r.h.s. of (11.1) for $d = 1, 2$) stems from the fact that the oscillatory integral approximating $e(x, x, \lambda, H_\alpha)$ (see equation (11.7)) contains no integration over x and therefore is more singular than the integrals approximating the local traces above (see section 5). More precisely, on the first step, in proving (11.6), we have to impose the condition

$$|\nabla_\xi h| \ \geq \ c \ > \ 0 \qquad \text{on } \mathcal{E}_\lambda$$

on the model problem which is stronger than the corresponding condition

$$|\nabla h| \ \geq \ c \ > \ 0 \qquad \text{on } \mathcal{E}_\lambda$$

which was used in theorem 7.1. Removing the former condition by scaling is harder than the latter.

Appendix: Stationary Phase Expansion

In this appendix we derive a stationary phase expansion for the integral

$$I(\lambda,\alpha) \;=\; \alpha^{-d}\int\!\!\int e^{i\phi/\alpha} b\, dt dy\ , \tag{A.1}$$

defined in (5.15)–(5.16). We have shown in the beginning of the proof of theorem 5.2 that the critical manifold of ϕ on $\operatorname{supp} b$ is

$$C_\lambda \;\equiv\; \{0\}\times\mathcal{E}_\lambda\ . \tag{A.2}$$

To compute the Hessian, ϕ'', of ϕ on C_λ we note that due to the initial condition $\phi\,\big|_{t=0}= 0$ we have

$$\partial^2_{yy}\phi \;=\; O(t)$$

on $\operatorname{supp} b$. This together with (5.22) and (5.24) yields

$$\phi'' \;=\; \begin{pmatrix} -\xi\cdot\nabla W & -\nabla h\\ -\nabla h & 0\end{pmatrix} + O(t)\ . \tag{A.3}$$

This expression shows that $\phi''|_{C_\lambda}$ is non-degenerate in the direction transversal to C_λ, i.e. on $N_\sigma = T_\sigma{}^d \ominus T_\sigma C_\lambda$, $\sigma\in C_\lambda$. The determinant of the restriction of $\phi''(\sigma)$ to N_σ, $\sigma\in C_\lambda$, is

$$\det{}_N(\phi'') \;=\; -|\nabla h|^2 \tag{A.4}$$

and the signature of this restriction, which is the difference between the number of positive and negative eigenvalues, is

$$\operatorname{sgn}_N(\phi'') \;=\; 0\ . \tag{A.5}$$

Denote by $\phi''(\sigma)^{-1}$ the inverse of the restriction of $\phi''(\sigma)$ to N_σ, $\sigma\in C_\lambda$. In what follows z stands for $(t,y)\in{}^{2d+1}$, σ is a point in C_λ and w, a point in $\mathcal{E}_\lambda$. We often identify $\sigma=(0,w)$ with w. The main result of this appendix is

Theorem A.1.

$$
\begin{aligned}
I(\lambda,\alpha) \;&=\; 2\pi\alpha^{1-d}\sum_{k=0}^{N-1} k!^{-1}\int_{\mathcal{E}_\lambda}\left[\left(-\frac{i}{2}\alpha L\right)^k (b\rho e^{i\theta/\alpha})\right]_{C_\lambda} |\nabla h|^{-2}dw \\
&\quad + O(\alpha^{N+1-d}) \ ,
\end{aligned}
\tag{A.6}
$$

where dw is the surface measure on $\mathcal{E}_\lambda$,

$$
L \;=\; \langle \phi''(\sigma)^{-1}\nabla, \nabla\rangle \ , \tag{A.7}
$$

with ∇ , the gradient in (t,y) , ρ is a smooth function on ^{2d} obeying

$$
\rho|_{\mathcal{E}_\lambda} \;=\; |\nabla h| \ . \tag{A.8}
$$

$$
\rho \text{ is independent of } \hat{\xi} \ , \tag{A.9}
$$

where $\hat{\xi} = \xi/|\xi|$, and for $\sigma \in C_\lambda$,

$$
\theta \;=\; \phi(z) - \phi(\sigma) - \frac{1}{2}\langle z-\sigma, \phi''(\sigma)(z-\sigma)\rangle \ . \tag{A.10}
$$

Proof. Since $\phi''(\sigma)$ is non-degenerate on N_σ , $\sigma \in C_\lambda$, one can apply a generalized stationary phase method (see e.g. [Meyer 1967, Chaz 1974]) in order to find an expansion of $I(\lambda,\alpha)$. We take a more explicit route by reducing the problem, with help of change of variables, to a standard stationary phase method.

Since by lemma A.1, the phase function ϕ has no critical points on $\operatorname{supp} b$ away from C_λ , it suffices to restrict our attention to a neighbourhood of C_λ . Thus in what follows we assume tacitly that the integration extends to a neighbourhood of C_λ . Hence we can pass from y to new coordinates (s,w) , where $s \in [-\varepsilon,\varepsilon]$ for some sufficiently small ε and $w \in \mathcal{E}_\lambda$, using the map $g:\ [-\varepsilon,\varepsilon]\times\mathcal{E}_\lambda \to {}^d$, defined by

$$
g(s,w) \;=\; w + s\nabla h(w) \ . \tag{A.11}
$$

Denote by dw a natural measure on $\mathcal{E}_\lambda$, then

$$
dy \;=\; \tilde{\rho}(s,w)ds dw \ , \tag{A.12}
$$

where $\tilde{\rho}$ is the absolute value of the Jacobian of the transformation (A.11). The function $\tilde{\rho}$ is smooth and has the following properties

$$\tilde{\rho}(s,w) = |\nabla h(w)| + O(s) \tag{A.13}$$

and

$$\tilde{\rho} \text{ is independent of } \hat{\xi} , \tag{A.14}$$

where $\hat{\xi} = \xi/|\xi|$. The first property is obvious, to explain the second one we notice that

$$\mathcal{E}_\lambda = F_\lambda \times S^{d-1} , \tag{A.15}$$

where $F_\lambda \subset {}^d \times {}^+$ is given by

$$F_\lambda = \{(x,k) \,|\, f(x,k) = \lambda\} \tag{A.16}$$

with

$$f(x,k) = \frac{1}{2}k^2 - W(x) . \tag{A.17}$$

Thus the natural measure on $\mathcal{E}_\lambda$ can be written as

$$d\omega = d\varphi d\theta , \tag{A.18}$$

where $d\varphi$ and $d\theta$ are the surface measures on F_λ and S^{d-1}, respectively. Transformation (A.11) can be written as

$$\begin{aligned} x &= \varphi_x + s\partial_x f(\varphi) \\ |\xi| &= \varphi_k + s\partial_k f(\varphi) \\ \hat{\xi} &= \theta , \end{aligned} \tag{A.19}$$

where $\varphi = (\varphi_x, \varphi_k) \in F_\lambda$ and $\theta \in S^{d-1}$. Consequently, the Jacobian of (A.11) is equal to the Jacobian of (A.19) and is therefore independent of $\hat{\xi}$.

Now make change of variables (A.11) in integral (A.1):

$$I = \alpha^{-d} \int\int\int e^{i\tilde{\phi}/\alpha} \tilde{b}\tilde{\rho} dt ds dw , \tag{A.20}$$

where the integration extends over $\times [-\varepsilon, \varepsilon] \times \mathcal{E}_\lambda$,

$$\tilde{\phi} \;=\; \phi \circ g \tag{A.21}$$

and

$$\tilde{b} \;=\; b \circ g \; . \tag{A.22}$$

Note that in a careful analysis we would have to split integral (A.1) into two integrals, one over a neighbourhood of C_λ and the other over the complement, then (A.20) would represent the former integral. Now we freeze the variable ω and consider the remaining integral

$$I_1(\lambda, \alpha, w) \;=\; \int\int e^{i\tilde{\phi}/\alpha} \tilde{b}\tilde{\rho} dt ds \; . \tag{A.23}$$

We want to apply a stationary phase expansion to this integral. This is possible due to

Lemma A.2. *Let $\nabla h \neq 0$ on $\mathcal{E}_\lambda$. Then for t sufficiently small and $w \in \mathcal{E}_\lambda$ fixed, $(0,0)$ is the only critical point of $\tilde{\phi}$. Moreover, this critical point is non-degenerate.*

The proof of this lemma is done similarly to the statement in the beginning of the proof of theorem 5.2 and of equations (A.3)–(A.4). We use that

$$\partial_t(\phi \circ g) \;=\; (\partial_t \phi) \circ g \tag{A.24}$$

$$\partial_s(\phi \circ g) \;=\; (\nabla h \cdot \nabla_y \phi) \circ g \; . \tag{A.25}$$

The first relation is straightforward, the second one uses that $\partial_k f \;=\; \partial_{|\xi|} h|_{|\xi|=k}$ and $\partial_{|\xi|} \;=\; \xi \cdot \partial_\xi$. We will not repeat the whole proof here but just write out some of the expressions:

$$\begin{aligned} -\partial_t \tilde{\phi} \;&=\; h \circ g - \lambda + O(t) \\ &=\; s|\nabla h(w)|^2 + O(s^2) + O(t) \; , \\ \partial_s \tilde{\phi} \;&=\; -|\nabla h(w)|^2 t + O(t^2) + O(ts) \end{aligned}$$

and

$$\tilde{\phi}'' \;=\; \begin{pmatrix} -\xi \cdot \nabla W & -|\nabla h|^2 \\ -|\nabla h|^2 & 0 \end{pmatrix} + O(t) \; . \tag{A.26}$$

Here and in what follows the leading term is evaluation on C_λ, i.e. at $t = s = 0$. In particular

$$\det \tilde{\phi}'' \;=\; -|\nabla h|^4 + O(t) \; . \tag{A.27}$$

Hence for t sufficiently small and all s

$$|\det \tilde{\phi}''| \;\geq\; \frac{1}{2}|\nabla h|^4 \;\geq\; \delta \;>\; 0 \; . \tag{A.28}$$

Due to lemma A.4 and equation (A.28) a stationary phase expansion (see [AsadaFuj 1978, Hörm I] is applicable to I_1 and yields

$$\begin{aligned} I_1(\lambda,\alpha,w) \;&=\; 2\pi\alpha|\det\tilde{\phi}''(w)|^{-\frac{1}{2}}e^{i\tilde{\phi}(w)/\alpha}e^{\frac{\pi i}{4}\operatorname{sgn}\tilde{\phi}''(w)} \\ &\times \sum_{k=0}^{N-1} k!^{-1}\left[\left(\frac{i}{2}\alpha\tilde{L}\right)^k \tilde{b}\tilde{\rho}e^{i\tilde{\theta}/\alpha}\right]_{t=s=0} + p_N \; , \end{aligned} \tag{A.29}$$

where $\operatorname{sgn} A$ is the difference between positive and negative eigenvalues of A,

$$\tilde{L} \;=\; \langle \tilde{\phi}''(w)^{-1}\partial, \partial\rangle \tag{A.30}$$

with $\partial = (\partial_t, \partial_s)$,

$$\begin{aligned} \tilde{\theta}(t,s,w) \;&=\; \tilde{\phi}(t,s,w) \\ &\quad - \frac{1}{2}\langle (t,s), \tilde{\phi}''(w)(t,s)\rangle \end{aligned} \tag{A.31}$$

and the remainder p_N is compactly supported in w and t and obeys the estimates

$$\partial^\beta p_N \;=\; O(\alpha^{N+1}) \; . \tag{A.32}$$

Now we compute

$$\tilde{\phi}(w) \;=\; 0 \; , \tag{A.33}$$

$$\operatorname{sgn}\tilde{\phi}''(w) \;=\; 0 \; , \tag{A.34}$$

$$\det\tilde{\phi}''(w) \;=\; -|\nabla h|^4 \; , \tag{A.35}$$

$$\tilde{\phi}''(w)^{-1} \;=\; \begin{pmatrix} 0 & -|\nabla h|^{-2} \\ -|\nabla h|^{-2} & \frac{\xi\cdot\nabla W}{|\nabla h|^4} \end{pmatrix} \; . \tag{A.36}$$

It is a simple exercise to check with help of (A.24) and (A.25) that

$$\tilde{L}(f \circ g) \;=\; (Lf) \circ g \;, \tag{A.37}$$

where $\tilde{L}$ and L are given by (A.30) and (A.7), respectively. Now we define ρ and θ through

$$\tilde{\rho} \;=\; \rho \circ g \tag{A.38}$$

and

$$\tilde{\theta} \;=\; \theta \circ g \tag{A.39}$$

and similarly for p_N. Substituting (A.33)–(A.39) into (A.29), taking into account that

$$f \circ g|_{t=s=0} \;=\; f|_{C_\lambda}$$

and integrating over $w \in \mathcal{E}_\lambda$, we arrive at (A.6).

Supplement

In this supplement we give a direct and elementary proof of theorem 7.5.

Theorem S.1. *Let* g *be a smooth and bounded function,* $O(\lambda^{-d-3})$ *as* $\lambda \to +\infty$ *together with its derivatives. Let* $\psi \in C_0^\infty\big(B(0,1)\big)$ *. Then*

$$\begin{aligned} \operatorname{tr}\big(\psi g(H_\alpha)\big) \;&=\; \alpha^{-d}\int\!\!\int \psi(x) g\big(h(x,\xi)\big)dxd\xi \\ &\quad + O(\alpha^{2-d}) \ . \end{aligned} \tag{S.1}$$

Proof. We use representation (7.1). Using a smooth partition of unity we split $g(\lambda)$ into a piece supported in $\lambda \le -\sup\limits_{B(0,2)} W - 1$ and one supported in $\lambda \ge -\sup_{B(0,2)} W - 2$. The latter piece is broken up again by applying a smooth partition of unity to its α-Fourier transform. As a result we achieve the decomposition

$$g \;=\; g_1 + g_2 + g_3 \ ,$$

where g_i are smooth and bounded, g_3 is supported in $(-\infty, -\sup\limits_{B(0,2)} W - 1]$, $g_2 = O(|\lambda|^{-d-3})$ as $|\lambda| \to \infty$ and its α-Fourier transform is supported in $\backslash(-\frac{1}{2}T, \frac{1}{2}T)$ and the α-Fourier transform of g_1 is supported in $[-T, T]$. Here $T > 0$ is sufficiently small (determined, essentially, by the existence interval for the underlying classical flow). We have

$$\|g_3(H)\psi\|_1 \;\le\; C\alpha^M \tag{S.2}$$

for any $M \ge 0$ due to theorem 4.4.

Next, we claim that

$$(H+i)^{d+2} g_2(H) \;=\; O(\alpha^M) \tag{S.3}$$

for any M . Indeed,

$$\begin{aligned} &(H+i)^m \int \hat{g}_2(-t)U(t)dt \\ =\; &\int \hat{g}_2(-t)(D_t + i)^m U(t)dt \\ =\; &\int \big((-D_t + i)^m \hat{g}_2(-t)\big)U(t)dt \ . \end{aligned}$$

Using this, we estimate for $m = d + 2$

$$
\begin{aligned}
& \|(H+i)^m g_2(H)\| \\
\leq \ & \frac{1}{2\pi\alpha} \int_{|t| > \frac{1}{2}\varepsilon} |\big((-D_t + i)^m \hat{g}_2^{\mathrm{normal}}\big)(-t/\alpha)| dt \\
\leq \ & C \int_{|t| \geq \frac{1}{2}\varepsilon} (|t|/\alpha)^{-M} dt \\
= \ & O(\alpha^M) \ ,
\end{aligned}
$$

for any $M \geq 0$, which yields (S.3). Estimate (4.5) together with equation (S.3) yields

$$
\|g_2(H)\psi\|_1 \ = \ O(\alpha^{M-d-\varepsilon}) \tag{S.4}
$$

Next, we proceed to the function g_1. Recall that $F(t)$ is the Fourier integral operator constructed in section 5. Pick up φ in the definition of $F(t)$ obeying $\varphi = 1$ on $(\operatorname{supp}\psi \times {}^{d}) \cap \operatorname{supp} g(h)$. Denote as before

$$
G(t) \ = \ U(t) - F(t)
$$

and write

$$
\begin{aligned}
g_1(H) \ = \ & \frac{1}{2\pi\alpha} \int \hat{g}_1(-t) F(t) dt \\
& + \frac{1}{2\pi\alpha} \int \hat{g}_1(-t) G(t) dt \ .
\end{aligned} \tag{S.5}
$$

By theorem 6.2, for N the same as in (5.6)

$$
\| \int \hat{g}_1(-t) G(t) dt \psi(x) \|_1 \ \leq \ C\alpha^{N-2d} \ . \tag{S.6}
$$

Now we study the first term on the r.h.s. of (S.5).

Lemma S.2.

$$
\begin{aligned}
& \operatorname{tr} \psi \int \hat{g}_1(-t) F(t) dt \\
= \ & 2\pi\alpha^{1-d} \int \int \psi g_1(h) dx d\xi + O(\alpha^{3-d}) \ .
\end{aligned} \tag{S.7}
$$

Proof. In this proof we omit the subindex 1 at g_1. Using the definition of $g(D_t)$ and the Plancherel formula, we obtain

$$
\begin{aligned}
& \int \hat{g}(-t) F(t) dt \\
& = 2\pi\alpha g(D_t) F(t) \big|_{t=0} \ .
\end{aligned} \tag{S.8}
$$

Remembering definition (5.1) of $F(t)$, we find

$$\begin{aligned} &\operatorname{tr}\psi \int \hat{g}(-t)F(t)dt \\ &= 2\pi\alpha^{1-d}\int\int \psi g(D_t)(ae^{i\phi/\alpha})\,\Big|_{t=0}\,dxd\xi\ , \end{aligned} \tag{S.9}$$

where, recall, $\phi = S - x\cdot\xi$. We claim that

$$\begin{aligned} g(D_t)(ae^{i\phi/\alpha})\,\Big|_{t=0} &= g(h)\varphi \\ &- \frac{1}{2}\alpha\varphi\xi\cdot\nabla W g''(h) + \alpha^2 r \end{aligned} \tag{S.10}$$

with r, a smooth and compactly supported symbol obeying

$$\int\int |r|dxd\xi \ \le\ C \tag{S.11}$$

with the constant independent of α. We prove this relation. First, using that $\phi\,\big|_{t=0} = 0$ and $a\,\big|_{t=0} = \varphi$, we expand in t:

$$\phi \ =\ t\phi_1 + t^2\phi_2 + t^3\phi_3$$

and

$$a \ =\ \varphi + tb_1 + t^2 b_2\ ,$$

where

$$\begin{aligned} \phi_1 &= \partial_t S\,\Big|_{t=0}\ , \\ \phi_2 &= \partial_t^2 S\,\Big|_{t=0}\ , \\ b_1 &= \partial_t a\,\Big|_{t=0} \end{aligned}$$

and ϕ_3 and b_2 are smooth functions on $[-T,T]\times B(0,2)\times B(0,K+3)$ with b_2 compactly supported in x and ξ. Combining these two expansions, we obtain

$$\begin{aligned} ae^{i\phi/\alpha} &= e^{i\phi_1 t/\alpha}(\varphi + tb_1 + t^2 i\varphi\phi_2/\alpha) \\ &+ e^{i\phi_1 t/\alpha}t^2\sum_{n=0}^{2}\left(\frac{t}{\alpha}\right)^n c_n\ , \end{aligned} \tag{S.12}$$

where c_n are smooth functions on $[-T,T]\times B(0,2)\times B(0,K+3)$, compactly supported in x and ξ. Using that

$$g(D_t)e^{i\phi_1 t/\alpha} \ =\ g(-\phi_1)e^{i\phi_1 t/\alpha} \tag{S.13}$$

and that

$$[g(D_t), t^n] = (i\alpha)^n g^{(n)}(D_t) + \sum_{m=1}^{n} O(t^m \alpha^{n-m}) \ , \tag{S.14}$$

we find

$$\begin{aligned} & g(D_t)(ae^{i\phi/\alpha}) \\ &= e^{k\phi_1 t/\alpha}[g(-\phi_1)\varphi - i\alpha g'(-\phi_1)b_1 - i\alpha g''(-\phi_1)\varphi\phi_2] \\ &\quad + \alpha^2 \sum_{n=2}^{4} (i)^n g^{(n)}(D_t)(c_n e^{id_1 t/\alpha}) \\ &\quad + \sum_{m=1}^{4} O(t^m \alpha^{2-m}) \ . \end{aligned} \tag{S.15}$$

By the Hamilton-Jacobi equation, $\phi_1 = -h(x,\xi)$ and by the definition of a and initial conditions (5.8), $b_1 = 0$. Using, in addition, (5.24), we conclude that

$$\begin{aligned} & g(D_t)(ae^{i\phi/\alpha}) \ \big|_{t=0} \\ &= g(h)\varphi + \frac{1}{2}\alpha\varphi\xi \cdot \nabla W g''(h) + \alpha^2 r \ , \end{aligned} \tag{S.16}$$

where

$$r = \sum_{n=2}^{4} (i)^n g^{(n)}(D_t)(c_n e^{-iht/\alpha}) \ \big|_{t=0} \ . \tag{S.17}$$

In order to estimate the last term we use the representation

$$g(D_t) = \frac{1}{2\pi\alpha} \int_{-\infty}^{\infty} \hat{g}(s) e^{isD_t/\alpha} ds \ , \tag{S.18}$$

where $\hat{g}(s)$ is the α-Fourier transform of g, and the fact that $e^{isD_t/\alpha}$ is a shift by s. This yields

$$\begin{aligned} & g^{(n)}(D_t)(c_n e^{-iht/\alpha}) \ \big|_{t=0} \\ &= \frac{1}{2\pi\alpha} \int \widehat{g^{(n)}}(s) e^{-ihs/\alpha} c_n(s,x,\xi) ds \ . \end{aligned} \tag{S.19}$$

Remembering now that $\hat{g}$ is supported in $[-T,T]$ and that

$$\begin{aligned} & \frac{1}{\alpha} \int |\widehat{g^{(n)}}(s)| ds \\ &= \int |s|^n |\hat{g}^{\text{normal}}(s)| ds \ < \ \infty \end{aligned}$$

and using that c_n are smooth and compactly supported in x and ξ, provided $|t| \leq T$, we derive (S.11). Thus (S.10)–(S.11) is proved.

Now, since $\varphi(x,\xi)$ and $h(x,\xi)$ are even in ξ, we have

$$\int \varphi\xi \cdot \nabla W g''(h) dx d\xi \;=\; 0 \,. \tag{$S.20$}$$

This together with (S.9)–(S.11) and the fact that $\varphi = 1$ on $(\operatorname{supp}\psi \times {}^{d}) \cap \operatorname{supp} g(h)$ yields (S.7).

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