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ASYMPTOTIC EXPANSIONS FOR QUANTUM MECHANICAL BOUND-STATE ENERGIES NEAR THE CLASSICAL LIMIT

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INTRODUCTION :

We investigate asymptotic expansions for the levels of

$$H(\hbar, m) = -\frac{\hbar^2}{2m}\Delta + V$$

in the limit $K^4 = \frac{\hbar^2}{2m} \longrightarrow 0$. Here V is a spherically symetric potential of the type encountered in molecular physics namely

(A) i) $V \in L$

ii) V has an absolute minimum V_0 for $X = X_0$, $X_0 \neq 0$.

iii) $V(X) = \sum_{n=0}^{N} a_n (X-X_0)^n + R_{N+1}(X)$ where $R_{N+1}(X) = O(X-X_0)^{N+1}$

as $X \longrightarrow X_0$, this expansion being on some interval J centered around X_0 .

iv) $\inf_{X \notin J} V(X) > V_0$.

This problem arises in connection with the semi-classical limit of quantum mechanics and also with the Born-Oppenheimer approximation [1].

That this perturbation problem is singular is well-known [2, 3] and can be seen very easily from the fact that the essential spectrum of $H(\hbar, m)$ is $[V_\infty, \infty)$ as long as $\frac{\hbar^2}{2m} \neq 0$ although the spectrum of the limiting operator V is usually continuous and consists of $[V_0, \infty)$.

Our method uses mainly the ideas of Maslov [3] and some recent estimates of B-Simon [4] on decay properties of eigenfunctions for Schrödinger operators supplemented by some suitable uniform estimates for families of the type encountered here.

Our result expressed in Theorems 1 and 2 below is that discrete levels of $H(\hbar, M)$ admit asymptotic expansions in the parameter

$$K = \left(\frac{\hbar^2}{2M}\right)^{1/4}$$

up to order N as expected from W.K.B. method or Born-Oppenheimer approximation.

We give prescriptions for the computation of terms in this expansion. In the case $N = 2$ we obtain the well-known harmonic approximation.

We will not be concerned in this paper about finding the best approximation scheme for levels of $H(K, M)$. In that respect the use of expansions in K does not necessarily leads to very good estimates ; however, they are interesting both from a practical and phenomenological point of view since perturbation coefficients can be easily calculated from the well-known harmonic oscillator eigenquantities and have in applications, e.g. molecular physics, direct physical interpretations.

II - THE MAIN THEOREMS

We refer to Kato [1] for the standard material used in this chapter on quadratic forms associated to Schrödinger operators. Let V satisfy assumptions (A) and t_1 be the associated closed symmetric quadratic form, densely defined on $L^2(\mathbb{R}^3)$

Let t_0 be the Dirichlet form associated to the usual self-adjoint extension of $-\Delta$ on $L^2(\mathbb{R}^3)$
Then $t(K) = K^4 t_0 + t_1$, $K > 0$, is defined, symmetric and closed on $Q(t_0) \cap Q(t_1)$, where $Q(\cdot)$ denotes the quadratic form domain. Obviously $Q(t(K)) \supset C_0^\infty(\mathbb{R}^3)$ so $t(K)$ is densely defined and since under our assumptions it is bounded below there exists a self-adjoint operator $H(K)$ associated to $t(K)$ such that $\forall \phi \in \mathcal{D}(H(K))$

$$H(K)\,\phi = -K^4 \Delta \phi + V\phi$$

One can show that

$$\sigma_e(H(K)) \subseteq [V_\infty, \infty)$$

where $V_\infty = \inf \lim\limits_{X \to \infty} V(X)$

Since V is spherically symmetric one can perform the usual angular momentum reduction ; then $t(K)$ is unitarily equivalent to the direct sum $\bigoplus_{\ell=0}^{\infty} \bigoplus_{m=-\ell}^{+\ell} \tilde{t}_\ell(K)$ where $\tilde{t}_\ell(K)$ is the closed quadratic form on $L^2(R^+)$ given by :

$$\tilde{t}_\ell(K) = K^4 d_0 + \tilde{t}_{1,\ell}(K)$$

where d_0 is the Dirichlet form on $L^2(R^+)$:

$$d_0[\varphi,\xi] = +\int_0^\infty \overline{\varphi'(x)}\,\xi(x)\,dx$$

with domain

$$\mathcal{Q}(d_0) = \left\{\varphi \in L^2(\mathbb{R}^+) ; \varphi' \in L^2(\mathbb{R}^+) \text{ and } \varphi(0) = 0\right\}$$

and

$$\tilde{t}_{1,\ell}(\kappa)[\varphi,\xi] = \int_0^\infty \overline{\varphi(x)}\left[\kappa^4 \frac{\ell(\ell+1)}{x^2} + V(x)\right]\xi(x)\,dx$$

where $Q(\tilde{t}_{1\ell})$ is defined in an obvious way. Both forms are closed, symmetric, densely defined and bounded below ; so one has

$$\mathcal{Q}(\tilde{t}_\ell(\kappa)) = \mathcal{Q}(d_0) \cap \mathcal{Q}(\tilde{t}_{1,\ell}(\kappa)) \quad \text{and } \tilde{t}_\ell(\kappa)$$

is closed on this domain. Let $\tilde{h}_\ell(\kappa)$ be the corresponding self-adjoint operator. The discrete spectrum $\sigma_d(H(\kappa))$ is related to the $\sigma_d(\tilde{h}_\ell(\kappa))$'s by

(1) $$\sigma_d(H(\kappa)) = \bigcup_{\ell,m} \sigma_d(\tilde{h}_\ell(\kappa))$$

To investigate the spectrum of $\tilde{h}_\ell(\kappa)$ let us write

$$L^2(\mathbb{R}) = L^2(-\infty, -\kappa^{-1}X_0) \oplus L^2(-\kappa^{-1}X_0, +\infty)$$

and consider the quadratic form

(2) $$t_\ell(\kappa) = \kappa^{-2}(V_\infty - V_0) \oplus [d_\kappa + t_{1,\ell}(\kappa)]$$

where $t_{1,\ell}(\kappa)$ is given by :

$$t_{1,\ell}(\kappa)[\varphi,\xi] = \int_{-\kappa^{-1}X_0}^\infty \overline{\varphi(x)}\,W_\ell(\kappa,x)\,\xi(x)\,dx$$

with

(3) $$W_\ell(\kappa,x) = \kappa^2 \frac{\ell(\ell+1)}{|X_0+\kappa x|^2} + \kappa^{-2}[V(X_0+\kappa x) - V_0]$$

and d_K is the Dirichlet form on $L^2(-\kappa^{-1}X_0, \infty)$. The form $d_\kappa + t_{1,\ell}(\kappa)$ is clearly obtained from $d_0 + \tilde{t}_{1,\ell}(\kappa)$ by the following canonical transformations :

1°) A coordinate transformation $X \longrightarrow X_0 + \kappa X$

2°) Substraction of the constant V_0

3°) Multiplication by κ^{-2}

From this it follows that the relation between eigenvalues $\tilde{E}_\ell(\kappa) \in \sigma_d(\hat{h}_\ell(\kappa))$ located below $\kappa^{-2}[V_\infty - V_0]$ (essential spectrum threshold for $\hat{h}_\ell(\kappa)$) and those $E_\ell(\kappa)$ of the self-adjoint operator $h_\ell(\kappa)$ associated to $t_\ell(\kappa)$ is

(4) $$\tilde{E}_\ell(\kappa) = V_0 + \kappa^2 E_\ell(\kappa)$$

since the coordinate transformation is implemented by a unitary operator

$$\varphi \in L^2(\mathbb{R}^+) \rightarrow \varphi_\kappa \in L^2(-\kappa^{-1}x_0, \infty) \text{ where}$$

(5) $$\varphi_\kappa(x) = \kappa^{1/2} \varphi(x_0 + \kappa x)$$

we can now state our main results:

THEOREM 1

Under assumptions (A) on V eigenvalues $E_\ell(\kappa)$ of $h_\ell(\kappa)$, $\ell = 0, 1, 2, \ldots$, have asymptotic expansions to order (N-2) given by the formal Rayleigh - Schrödinger perturbation series for the operator on $L^2(R)$:

(6) $$h_\ell^{(N)}(\kappa) = -\frac{d^2}{dx^2} + W_\ell^{(N)}(\kappa)$$

where $W_\ell^{(N)}(\kappa)$ is the sum of the terms of degree $\leq N - 2$ in the K - expansion around 0 of $W_\ell(\kappa)$.

REMARK :

It is important here to notice that the operators $h_\ell^{(N)}(\kappa)$ are not self-adjoint if $W_\ell^{(N)}(\kappa)$ is not an even polynomial. However, it is always possible to compute Rayleigh - Schrödinger coefficients formally from the unperturbed

(7) $$h_\ell^{(2)} = h = -\frac{d^2}{dx^2} + W^{(2)}$$

where
$$W^{(2)} = x^2 V''(x_0)$$

On the other hand since obviously only even powers of K appear in the expansion of eigenvalues, one can restrict oneself to the consideration of even N's only so that this mathematical problem does not arise ($W_\ell^{(N)}(\kappa)$ is then an

even polynomial in K).
Concerning eigenvalues and eigenvectors of $H(\kappa)$ one has :

THEOREM 2 -

Under assumptions (A) on V, eigenvalues $\widetilde{E}_\ell(\kappa)$ of $H(\kappa)$ corresponding to a total angular momentum ℓ have asymptotic expansions to order N.
These expansions are given in terms of those for $E_\ell(\kappa)$ by the relation :

$$\widetilde{E}_\ell(\kappa) = V_0 + \kappa^2 E_\ell(\kappa)$$

REMARKS :

a) This theorem is an immediate consequence of theorem 1 and the angular momemtum reduction procedure that we have performed leading to the relation (1)

b) For N = 2 one obtains in particular the so-called harmonic approximation

$$\widetilde{E}_\ell(\kappa) = V_0 + \kappa^2(2n+1)\,\omega + O(\kappa^3) \quad (\kappa \to 0) \tag{8}$$

where n can take any positive ~~integer/~~value.
For N = 3 the correction of order 3 to $\widetilde{E}_\ell(\kappa)$ vanishes for symmetry reasons (eigenvectors of h have a definite parity). As indicated before this will then be the case for all corrections of odd order.
For N = 4 one obtains an expansion

$$\widetilde{E}_\ell(\kappa) = V_0 + \kappa^2(2n+1)\omega + \kappa^4\left[\frac{\ell(\ell+1)}{X_0^2} + \delta_n\right] + O(\kappa^5) \; (\kappa \to 0)$$

where δ_n is an anharmonic correction which can be easily explicited. If one takes $\delta_n = 0$ one obtains the so called Born-Oppenheimer approximation.

If N can be taken arbitrarily large, as is the case in some specific examples of molecular physics one gets asymptotic expansions to any order.

c) In the course of the demonstration of Theorem 1, one shows that if $\varphi_{\ell,\kappa}$ is an eigenfunction associated to an eigenvalue of the form (8) then supp $\varphi_{\ell,\kappa} \subset [\varepsilon\kappa^{-1}X_0, \infty)$ and $\varphi_{\ell,\kappa}$ converges strongly to the n^{th} excited state of the harmonic oscillator operator (7). This fact, together with the relation (5) between $\varphi_{\ell,\kappa}$ and the radial part of the associated eigenfunction $\psi_{\ell m,\kappa}$ in $L^2(R^3)$ for $H(\kappa)$

giving :

(9) $$\Psi_{\ell m,\kappa}(X,\theta,\varphi) = \kappa^{-1/2}\, X^{-1}\, \varphi_{\ell,\kappa}(\kappa^{-1}(X-X_o))\, Y_{\ell m}(\theta,\varphi)$$

shows that $\Psi_{\ell m,\kappa}$ is more and more concentrated around $X = X_o$ as can be expected from the fact that in the classical limit $K = 0$ the particle stays at these extremal positions minimizing the classical energy (with V_o as a minimal value).

Proof of Theorem 1

For convenience of notations we will now drop the index ℓ.
An essential step in the proof will be the stability of eigenvalues for the unperturbed operator h under the perturbation $h(K) - h$, namely the fact that for K sufficiently small a given neighborhood of contains one and only one eigenvalue of $h(K)$. As shown in [2] this will be a consequence of the following

Proposition I -

Let z, $\operatorname{Im} z \neq 0$. Then $R(z, K) = (h(K) - z)^{-1}$ converges in the norm topology of operators to $R_h(z) = (h - z)^{-1}$

Proof :

Let $\varepsilon > 0$ and define an interval I_ε centered around X_o by

$$|V(X_o+X) - V(X_o) - X^2 V''(X_o)| < \varepsilon X^2 \qquad \forall X \in I_\varepsilon$$

Then $\forall \kappa > 0$

$$|W_\kappa(X) - X^2 V''(X_o)| < \varepsilon X^2 + \delta \kappa^2 \quad \text{on } \kappa^{-1} I_\varepsilon$$

where δ is a constant.
Let us write a smooth partition of the identity on R.

$$1 = \chi_-(\kappa) + \chi(\kappa) + \chi_+(\kappa)$$

where $\chi(K)$ (resp. $\chi_-(\kappa)$, $\chi_+(\kappa)$) is a smoothened characteristic function for $K^{-1} I$ (resp. for the half-line on the left and right of $K^{-1} I_\varepsilon$). Then one can write :

$$\| R(z,\kappa) - R_h(z) \| \leq \| R(z,\kappa)(\chi_-(\kappa) + \chi_+(\kappa))\| + \| R_h(z)(\chi_-(\kappa) + \chi_+(\kappa))\| + \| (R(z,\kappa) - R_h(z))\, I(\kappa)\| \tag{10}$$

The two first terms of the r.h.s. of (10) tend to zero ; this comes from the fact that both resolvents are of the form $(A + W - z)^{-1}$, $\mathrm{Im}\, z \neq 0$, where A and W are non negative operators and

$$n\cdot\lim_{\kappa \to 0} \sqrt{W}\cdot \chi_\pm(\kappa) = 0$$

Then using the fact, proved in App. I that $\| (A + W - z)^{-1}\sqrt{W}\|$ is bounded one gets the desired result. The analysis of the last term in (10) uses the estimate (9) ; write

$$\begin{aligned}(R(z,\kappa) - R_h(z))\,\chi(\kappa) &= R(z,\kappa)\,(W(\kappa) - X^2 V''(X_0))\,\chi(\kappa)\, R_h(z) \\ &\quad + [R(z,\kappa) - R_h(z)]\left(2\frac{d}{dX}\cdot\chi'(\kappa) + \chi''(\kappa)\right) R_h(z)\end{aligned} \tag{11}$$

where we have used the identity

$$[(A - z)^{-1}, B] = (A - z)^{-1}\,[B, A]\,(A - z)^{-1} \tag{12}$$

The first term on the r.h.s. of (11) is bounded by $\varepsilon \| X^2 R_h(z)\| + \delta'\kappa^2$. On the other hand, the characteristic functions of the supports of $I'(K)$ and $I''(K)$ tend strongly to zero and since $R_h(z)$ is compact, their products tend in norm to zero ; then it is enough to show that $\| R(z,\kappa)\frac{d}{dX}\cdot\chi'(\kappa)\|$ and $\| R_h(z)\,\chi''(\kappa)\|$ are bounded. This can be shown e.g by using the closed graph theorem for the adjoints and the technique of App. I .
Finaly the l.h.s. of (10) is bounded by $\varepsilon \| X^2 R_h(z)\| + O(\kappa)\ (\kappa \to 0)$
Since ε can be taken arbitrarily small and $\| X^2 R_h(z)\|$ is bounded (a simple exercise) the proof is complete.
Stability of eigenvalues will play an important role in the foregoing discussion. However, despite this, the Rayleigh-Schrödinger perturbation method cannot be applied directly to the perturbation h (K) - h for many reasons e.g. :

1) The difference between h and the $L^2(-\infty, -K^{-1}X_o)$ component of h (K) is never "small" ;

2) W(K) has a singularity at $X = -K^{-1}X_o$ and unperturbed eigenvectors of h are not in $\mathcal{D}(W(K))$

3) W (K) does not admit a regular perturbation expansion in K.
(The expansion around X_o is valid only locally and the coefficients are polynomials in X that is non small perturbations of h).

We will see that all these points can be taken care of by using decay properties of eigenfunctions as expressed by proposition 2 below. According to them one expects that only the part of W(K) wher the wave-functions are non-negligible should contribute significantly and one should be able to replace W(K) by regular perturbations for which Rayleigh-Schrödinger perturbation series make sense. It will remain to show that such series are precisely those obtained from the formal power series expansion of W (K) in K.
Existence of such regular perturbations will be a consequence of the uniform estimates provided by the next proposition.

PROPOSITION 2 :

Let $\varphi(K)$ be a normalized eigenvector of h(K) associated to an eigenvalue E(K). Assume that $E(K) \xrightarrow[K\to 0]{} \Lambda \in \sigma_d(h)$. Then for K sufficiently small :

i) $\mathrm{Supp}\, \varphi(K) \subset [K^{-1}X_o, \infty)$ and $\left(-\frac{d^2}{dX^2} + W(K)\right)\varphi(K) = E(K)\varphi(K)$

ii) Let $U(\alpha, K)$, $\alpha \in \mathbb{R}$, be the unitary group of multiplication by $\exp(i\alpha \int_o \sqrt{W(K,X)}\, dX$. Then the family $\{U(\alpha, K)\varphi(K)\}$ has an analytic extension to the ball $|\alpha| < 1$ which is uniformly bounded in K.

Proof :

i) is a consequence of the decomposition (2) and the fact that since $K^{-2}[V_\infty - V_o] \xrightarrow[K\to 0]{} \infty$ the component of $\varphi(K)$ in $L^2(-\infty, -K^{-1}X_o)$ must vanish for K sufficiently small.

To prove ii) let us first paraphrase Simon [4] to show that $U(\alpha, K)\,\varphi(K)$ can be analytically continued to the ball $|\alpha| < 1$.

Consider the family

$$h(K,\alpha) = U(K,\alpha)\, h(K)\, U^{-1}(K,\alpha) \tag{13}$$

A simple calculation shows that $h(K,\alpha)$ is the self-adjoint operator associated to the quadratic form (see (2))

$$t(K,\alpha) = t(K) - \alpha^2 t_1(K) - i\alpha\, t_2(K) \tag{14}$$

where

$$t_2(K)[\varphi,\xi] = 2\,\mathrm{Re} \int_{-K^{-1}X_0}^{\infty} \sqrt{W(K)}\; \bar{\varphi}(x)\, \xi'(x)\, dx$$

If in (14) we now let α be complex it is easy to see that for $|\alpha| < 1$ one has $Q(t(K,\alpha)) = Q(t(K))$ and $t(K,\alpha)[\varphi,\varphi]$ is analytic in K in that domain for $\varphi \in Q(t(K))$.

So $t(K,\alpha)$ is analytic of type (a) [2] and accordingly $h(K,\alpha)$ is a holomorphic family. From analytic perturbation theory [2] we can deduce that the eigenprojectors $P(K,\alpha)$ associated to the eigenvalue $E(K)\ (\in \sigma(h(K,\alpha))\ \forall \alpha)$ are analytic as long as $|\alpha| < 1$ (and $E(K)$ is not absorbed by the essential spectrum of $h(K,\alpha)$ which does not happen for K sufficiently small and $|\alpha| < 1$). From this and the fact that $P(K,\alpha)$ is a one dimensional projection operator having $U(\alpha, K)\,\varphi(K)$ as an eigenvector for α real follows the assertion that this vector has an analytic extension. To show uniform boundedness in the ball $|\alpha| < 1$ of the family $P(K,\alpha)$ it is enough to show that

$$n\text{-}\lim_{K \to 0} P(K,\alpha) = P(\alpha) \qquad \forall \alpha,\ |\alpha| < 1. \tag{15}$$

where $P(\alpha)$ is the eigenprojection for the eigenvalue $\Lambda \in \sigma_d(\alpha)$, $|\alpha| < 1$, with

$$h(\alpha) = -\frac{d^2}{dx^2} + i\alpha\left(x \cdot \frac{d}{dx} + h.c.\right) + (1-\alpha^2)\,x^2$$

This in turn is a consequence of the norm resolvent convergence

$$n \cdot \lim_{K \to 0} (h(K,\alpha) - z)^{-1} = (h(\alpha) - z)^{-1}$$

which can be shown along the same lines as Prop. 1 modulo some elementary modifications due to the non self-adjoint character of these new operators.
From (15) and Banach Steinhauss theorem one can deduce that the family is uniformly bounded in $|\alpha| < 1$ for K sufficiently small which shows part ii) of Prop. 3.
We now define regularisations to order (N-2) of W(K) as follows : under assumptions (A) on V it is not difficult to see that W (K) admits an expansion

(16) $$W(K,X) = \sum_{n=0}^{N-2} K^n P_n(X) + R_N(K,X)$$

where P_n is a polynomial with degree n+2 (in particular $P_o = X^2 V''(X_o)$) and

(17) $$|R_N(K,X)| \leq K^{N-1} Q(X) \quad , \quad X \in K^{-1} I$$

where I is the interval $J - X_o$ and Q is a polynomial of degree N + 1. Let

(18) $$W_r^{(N)}(K,X) = X^2 V''(X_o) + \sum_{n=2}^{N-2} K^n P_n(X) \chi(K,X)$$

where χ (K) is a smooth characteristic function for the interval $K^{-(1-\delta)}I$, $0 < \delta < 1$. The operator

(19) $$h_r^{(N)}(K) = -\frac{d^2}{dX^2} + W_r^{(N)}(K)$$

is obviously self-adjoint with the same domain as h. One can show the norm resolvent convergence of $h^{(N)}$(K) to h along the lines of Prop. 1 or more directly by noticing that for Im Z $\neq$ 0

(20) $$(h_r^{(N)}(K) - z)^{-1} - (h - z)^{-1} = (h_r^{(N)}(K) - z)^{-1} \left(\sum_{n=2}^{N-2} K^n P_n \chi(K) \right) (h - z)^{-1}$$

Since $d(P_n) = n + 2$ and $|K\dot{X}|$ is $O(K^{\delta})$ on supp $\chi(K)$ one has

$$\sup_X \left| K^n P_n(X)(1+X^2)^{-1} \chi(K,X) \right| = O(K^{n\delta}) \quad (K \to 0)$$

On the other hand $(1 + X^2)(h - z)^{-1}$ is bounded so that the proof of the norm convergence to zero of (20) can be easily completed. We are now ready to show that $W_\ell^{(N)}(K)$ is a good substitute for $W(K)$:

PROPOSTITION 3

Let $(E^{(N)}(K))$ (resp. $(E(K))$) be a family of eigenvalues of $h_\ell^{(N)}(K)$ (resp. $h(K)$) such that

$$\lim_{K \to 0} E^{(N)}(K) = \lim_{K \to 0} E(K) = \Lambda \in \sigma_d(h)$$

Let $(P^{(N)}(K))$ (resp. $(P(K))$) be the corresponding eigenprojectors. Then

i) $\operatorname{tr}((h_\ell^{(N)}(K) - h(K))P(K)) = O(K^{N-1}) \quad (K \to 0)$

ii) $E(K) - E^{(N)}(K) = O(K^{N-1})$ —

iii) $\|(1 - P^{(N)}(K))P(K)\| = O(K^{N-1})$ —

Proof :

To prove i) we denote by $\varphi(K)$ a normalized eignevector of the one dimensional projection operator $P(K)$. We have to estimate the expectation value $(\varphi(K) | h_\ell^{(N)}(K) - h(K) | \varphi(K))$

which is equal to $(\varphi(K) | W_\ell^{(N)}(K) - W(K) | \varphi(K))$ for K sufficiently small according to Prop. 2 i). This last quantity equals $(\varphi(K) | R_N(K)\chi(K) | \varphi(K))$

where R_N is defined in (16). According to (17) the first term is bounded by

$K^{N-1}(\varphi(K) | C\varphi(K))$ hence uniformly bounded by prop 2 ii) and assumption A4) on V which imply uniform exponential decay for the functions $\varphi(K)$.
As to the second term one can rewrite it as

$$|E(K) - z|^2 \left((1-\chi(K))\varphi(K) \,|\, (h(K)-\bar{z})^{-1} W(K) (h(K)-z)^{-1} \varphi(K)\right);$$

the middle operator is bounded by App. 1 and $\|(1-\chi(K))\varphi(K)\| = O(e^{-aK^{-1}}) \ (a > 0)$

by the uniform exponential decay property. This shows i).
Let us now write for Im $z \neq 0$:

$$(21) \quad E(\kappa) - E^{(N)}(\kappa) = (E^{(N)} - z)(E(\kappa) - z)\left(\varphi^{(N)}(\kappa) \mid \varphi(\kappa)\right)^{-1} \times \left(\varphi(\kappa) \mid R^{(N)}(z,\kappa) - R(z,\kappa) \mid \varphi(\kappa)\right)$$

where $R^{(N)}(z,\kappa) = \left(h^{(N)}(\kappa) - z\right)^{-1}$ and

$\varphi^{(N)}(\kappa)$ is a normalized eigenvector of the one dimensional projection operator $P^{(N)}(K)$; it can be choosen so that $\| \varphi^{(N)}(\kappa) - \varphi(\kappa) \| \underset{\kappa \to 0}{\longrightarrow} 0$.
It is then sufficient to show that the last factor on the r.h.s. of (21) is $O(K^{N-1})$. This can be done along the lines used in the proof of Prop. 1 by inserting a decomposition of the identity

$$I = \chi(\kappa) + (I - \chi(\kappa))$$

in front of $\varphi(K)$. The term $(I - \chi(\kappa))$ gives a contribution $O(e^{-aK^{-1}})$.
For the term $\chi(\kappa)$ we use an identity analogous to (11):

$$(22) \quad R^{(N)}(z,\kappa) - R(z,\kappa) = R^{(N)}(z,\kappa)\left(W(\kappa) - W_2^{(N)}(\kappa)\right)\chi(\kappa)\, R(z,\kappa) + \left(R^{(N)}(z,\kappa) - R(z,\kappa)\right)\left(2\frac{d}{dx} \cdot \chi'(\kappa) + \chi''(\kappa)\right) R(z,\kappa).$$

The second term on the r.h.s. of (22) gives a contribution $O(e^{-aK^{-1}})$. The first one gives a contribution

$$\left(\varphi^{(N)}(\kappa) \mid R_N(\kappa)\, \chi(\kappa) \mid \varphi(\kappa)\right)$$

which can been shown as above to be $O(K^{N-1})$.

We now prove iii) inductively assuming it is true for the (n - 1) lowest levels
Let $E_n^{(N)}(\kappa) \in \sigma_d(h_2^{(N)}(\kappa))$ and $E(\kappa) \in \sigma_d(h(\kappa))$
converge to the $n^{\underline{th}}$ eigenvalue of h. One has

$$(23) \quad \mathrm{tr}\left(\left(h_2^{(N)}(\kappa) - h(\kappa)\right) P(\kappa)\right) = \sum_j \left(E_j^{(N)} - E(\kappa)\right) \mathrm{tr}\left(P_j^{(N)}(\kappa)\, P(\kappa)\right)$$

Due to stability one can choose K sufficiently small so that

$$|E_j^{(N)}(K) - E(K)| > \delta > 0 \quad \text{for } j \neq n$$

On the other hand, by the induction hypothesis and the fact that $P^{(N)}(K)$ and $P(K)$ are one-dimensional projection operators one has

$$\mathrm{tr}(P_j^{(N)}(K)\, P(K)) = \| P_j^{(N)}(K)\, P(K) \| = O(K^{N-1}) \text{ for } j < n$$

This together with (ii) implies that in the sum on the r.h.s, of (23) the terms with $j \lesssim n$ give a contribution which is $O(K^{N-1})$. Since the remaining terms are positive one gets according to i)

$$(24) \quad \sum_{j \neq n} \mathrm{tr}(P_j^{(N)}(K)\, P(K)) \leq \delta^{-1} \sum_{j > n} (E_j^{(N)}(K) - E(K))\, \mathrm{tr}(P_j^{(N)}(K)\, P(K)) + \alpha K^{(N-1)}$$
$$= O(K^{N-1})$$

Now one has

$$\sum_{j \neq n} \mathrm{tr}(P_j^{(N)}(K)\, P(K)) = \| (1 - P_n^{(N)}(K))\, P(K) \| = O(K^{N-1})$$

from which iii) results according to (24).

According to Prop. 3 if the levels of h (K) have asymptotic expansions up to order N-2 they will coincide with those of $h_r^{(N)}(K)$. To complete the proof of our main theorems it is then sufficient to prove

PROPOSITION 4

Eigenvalues of $h_r^{(N)}(K)$ have asymptotic expansions to order N-2 given by the formal Rayleigh-Schrödinger perturbation series for the operator

$$h^{(N)}(K) = -\frac{d^2}{dX^2} + W^{(N)}(K)$$

where $W^{(N)}(K)$ is the sum of the terms of degree $\leqslant$ N-2 in the K-expansion (16) of W (K).

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Proof :

Assume $E^{(N)}(K) \xrightarrow[K\to 0]{} \Lambda$ and let Ω be the corresponding normalized eigenvector $h\,\Omega = \Lambda\,\Omega$. One has

$$E^{(N)}(K) = (h_2^{(N)}(K)\,\Omega \mid P^{(N)}(K)\,\Omega) / (\Omega \mid P^{(N)}(K) \mid \Omega)$$

It is enough to show that $h_2^{(N)}(K)\,\Omega$ and $P^{(N)}(K)\,\Omega$ have asymptotic expansions to order N-2 whose coefficients are just those obtained from the formal expansion (16) for W (K). More precisely we will see that the removal of in the expression (18) for $W_2^{(N)}(K)$ gives a contribution $O(K^{N-1})$ $(K \to 0)$. This is obvious for $h_2^{(N)}(K)\,\Omega$ since Ω is an Hermite function having e^{-ax^2}, $a>0$, decay so that

$$\| X^p (1-\chi(K))\,\Omega \| = O(\exp(-bK^{-2(1-\delta)}))$$

for some $a > 0$ and $\forall$ integer p.
Let us investigate $P^{(N)}(K)\,\Omega$. For this we use the representation

$$P^{(N)}(K) = \frac{1}{2i\pi} \int_C R^{(N)}(z,K)\, dz$$

where C is some contour enclosing Λ and $E^{(N)}(K)$ and no other point in $\sigma_d(h_2^{(N)}(K))$ or $\sigma_d(h)$. Iterating (N-2) times the second resolvent equation one gets

$$(25) \quad 2i\pi\, P^{(N)}(K)\,\Omega = \sum_{j=1}^{N-2} \int_C R_h(z)\,(W_2^{(N)}(K)\, R_h(z))^j\, \Omega\, dz$$
$$+ \int_C R_h(z)\,(W_2^{(N)}(K)\, R_h(z))^{N-2}\, W_2^{(N)}(K)\, R^{(N)}(z,K)\,\Omega\, dz$$

Terms appearing in the sum on the r.h.s. of (25) give contributions of the form

$$(26) \quad \gamma_n K^n \int_C R_h(z)\, X^p \chi(K)\, R_h(z)\, X^q \cdots X^\ell \chi(K)\, R_h(z)\, \Omega\, dz$$

with $n = p+q+\cdots+\ell \leq N-2$

Since $R_h(z)$ leaves $\mathcal{D}(e^{-\theta x^2})$ invariant ($0 < \theta < a$) (as can be shown e.g. using the techniques of Prop. 2), the removal of χ (K) in (26) will give a correction $O(\exp(-bK^{-2(1-\delta)}))$. Terms from the last integral on the r.h.s. of (25) have a similar structure but with the last resolvent replaced by $R^{(N)}(z, K)$ so that the above argument does not apply directly to show that they are $O(K^{N-1})$. But here it is enough to establish that coefficients of the K^n ' s in the contour integral are bounded uniformly in K and $z \in C$; this can be done using two tricks :

First use the relation (12) , to push the monomials to the right and make them act directly on Ω ; One can justify this procedure rigorously by a simple but lenghty domain analysis. Second use Banach-Steinhaus theorem to show that the resulting operators on the left of vectors $X^\alpha \Omega$ are bounded uniformly in K and $z \in C$. These operators are products of factors like $A\, R(z)\, B$ where $A = -\frac{i\,d}{d\,x}$ or 1 ; $B = \chi(K)$ or 1 and $R(z)$ is the resolvent of $h_\ell^{(N)}(K)$ or h. Using the result of App. I one can deduce that such operators are uniformly bounded in K and Z

Appendix 1 -

Let A and B be positive self-adjoint operators associated to quadratic forms t_A and t_B. Assume that $Q(t_A) \cap Q(t_B)$ is dense and let A + B be the self-adjoint operator associated to $t_A + t_B$. Then for all z in the resolvent set of A + B the operator $\sqrt{A}\,(A + B - z)^{-1}$ is bounded.

Proof :

$\forall \varphi$ one has

$$(\varphi \,|\, (A+B-\bar{z})^{-1} A (A+B-z)\varphi) \leq (\varphi, (A+B-\bar{z})^{-1}\varphi) + |z|\, \|(A+B-z)^{-1}\varphi\|^2$$

Since the L.h.s. is just $\|\sqrt{A}\,(A+B-z)^{-1}\varphi\|^2$ one gets

$$\|\sqrt{A}\,(A+B-z)^{-1}\| \leq (1+|z|)/\operatorname{dist}(z,\sigma(A+B))$$

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