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Pointwise Bounds on Eigenfunctions and Wave Packets in N-Body Quantum Systems

V. Lower Bounds and Path Integrals*

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Abstract. By using Agmon's geodesic ideas to single out particular regions in path space, we obtain optimal lower bounds on the leading behavior for the fall off of the ground state of multiparticle system.

1. Introduction

This paper is a contribution to the large literature on the decay at infinity of eigenvectors of Schrödinger operators, $-\frac{1}{2}\Delta + V$, associated to discrete spectrum [1, 3–5, 9, 12, 15, 17, 22–24, 27, 28, 32, 34, 37, 39, 46–48, 51]. For the *leading* behavior of the *ground state*, φ, our results are definitive in the sense that we will show that:

$$\lim_{|x|\to\infty} -[\log\varphi(x)]/\varrho(x) = 1 \tag{1.1}$$

for an explicit function ϱ and for a large class of potentials, V, including general N-body systems. The upper bounds implicit in (1.1) are not new: for multiparticle systems, they were found in successively more general cases by Mercuriev [37] (three-body), Deift et al. [17], and Hoffman-Ostenhoff et al. [4] (atoms with infinitely heavy nucleus) and Agmon [1] in the general case; for potentials going to infinity at infinity they were found by Lithner [34] and rediscovered by Agmon [1]. The Lithner-Agmon upper bounds are only proven to hold in some average sense, but it is easy to get pointwise bounds with minor extra restrictions on V (see Appendix 2). Our primary goal here will be to find lower bound complementary to these various upper bounds which show that the upper bounds are "best possible".

A major source of motivation for the approach we use is the part of Agmon's work [1] which identifies the function ϱ in (1.1). Let us initially describe the situation for the case $V\to\infty$, $V\geqq 1$ and continuous, a case treated by Lithner, with a related intuition.

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Agmon finds a sufficient condition for:

$$|\varphi(x)| \leqq c_\varepsilon e^{-(1-\varepsilon)\varrho(x)} \tag{1.2}$$

for all $\varepsilon > 0$ is that:

$$\tfrac{1}{2}|(\nabla\varrho)(x)|^2 \leqq V(x). \tag{1.3}$$

Related conditions were found using the Combes-Thomas method [15], in [48, 17], and using one of Agmon's ideas and the Combes-Thomas method we show that (1.3) implies (1.2) in Appendix 1. The main point for us is Agmon's analysis of (1.3). Let $\gamma(s)$ be a path from 0 to x. Then:

$$\begin{aligned}\varrho(x)-\varrho(0) &= \int_0^{s_0} \frac{d}{ds}\varrho(\gamma(s))ds \\ &= \int_0^{s_0} [\nabla\varrho](\gamma(s))\cdot\dot\gamma(s)ds \\ &\leqq \int_0^{s_0} \sqrt{2V(\gamma(s))}|\dot\gamma(s)|ds\end{aligned}$$

if (1.3). Thus, if (1.3) holds, and ϱ is normalized by $\varrho(0)=0$, then:

$$\varrho(x) \leqq \inf\left\{\int_0^{s_0} \sqrt{2V(\gamma(s))}|\dot\gamma(s)|ds;\ s_0 \geqq 0,\ \gamma(0)=0,\ \gamma(s_0)=x\right\}. \tag{1.4}$$

All the trial paths we use are implicitly assumed to have an almost everywhere derivative in L^1-sense. The right hand side of (1.4) is recognized as the geodesic distance $d(x,0)$ from x to 0 in the Riemannian metric with infinitesimal length $\sqrt{2V(x)}dx^2$ with dx^2 the usual Euclidean metric. Moreover, $d(x,0)$ obeys (1.3) [at least formally; $d(x,0)$ may not be C^1; see Appendix 1] since:

$$|d(x+\delta x,0)-d(x,0)| \leqq d(x+\delta x,x) \sim \sqrt{2V(x)}\delta x + O(\delta x^2).$$

Thus the choice $\varrho(x)=d(x,0)$ in (1.3) is optimal and henceforth we make this choice. We will call $\varrho(x)$ the *Agmon metric* [occasionally we use this term also for the underlying Riemannian structure $\sqrt{2V(x)}dx^2$, using a standard abuse of notation].

The occurrence of a geodesic distance in (1.4) is screaming out for some kind of path integral interpretation, suggesting that the approach of [12] can be extended to get best possible bounds. This is especially attractive for lower bounds since typically, it is much easier to get lower bounds in path integrals because one needs only to identify the relevant piece of path space and control its contribution to the path integral; moreover, Jensen's inequality often provides lower bounds on the portion of path space.

There is one immediate problem with this idea: path length is independent of parametrization so that minimizing paths in the variational principle (1.4) do not come with a unique parametrization, but contributions to path integrals do depend on parametrizations, so there is a problem in deciding what path minimizing (1.4) to pick as a "center" of a significant neighborhood in path space. The solution of this problem is quite interesting: the minimization problem for the lower bound in (1.1) is distinct from the problem (1.4) and this new function to be minimized will depend on parametrization; however the minimum value will be the same value as the minimum of the function on the right side of (1.4)!

To see the minimizing problem which will arise, let us rewrite the Feynman-Kac formula [49]:

$$\varphi(x)=\mathbf{E}\left\{\varphi(x+b(t))\exp\left[\int_0^t [E-V(x+b(s))]ds\right]\right\} \tag{1.5}$$

formally as:

$$\varphi(x)=N^{-1}\int \varphi(\gamma(t))\exp\left[-\tfrac{1}{2}\int_0^t |\dot\gamma(s)|^2 ds-\int_0^t V(\gamma(s))ds\right]e^{Et}\text{“}d\gamma\text{”}$$

with N and “$d\gamma$” formal objects and with a boundary condition $\gamma(0)=x$. Imagining that we want to consider paths with $\gamma(t)\approx 0$ so that $\varphi(\gamma(t))$ is not too small and ignoring the e^{Et} term, the natural function we want to minimize is [subject to $g(0)=x$ and $g(t)=0$]:

$$\mathscr{A}(g)=\tfrac{1}{2}\int_0^t |\dot g(s)|^2 ds+\int_0^t V(g(s))ds. \tag{1.6}$$

The pleasant fact is that the minimum of $\mathscr{A}(\cdot)$ is the same as the minimum of the right hand side of (1.4)! This is a small extension of the well known fact [21, 31] that classical paths [(1.6) is a classical action for a force ∇V, **not** $-\nabla V$] are geodesics in $\sqrt{E-V(x)}dx^2$ metric; not only are the paths as geodesics but the action is related to geodesic distance.

The details of this argument for the case $V\to\infty$ are given in Sect. 2; we learned from Tom Spencer that independently of our work, he has developed similar ideas and results by a closely related method [52].

We note that this is not the first time that geodesics have appeared in the context of path integrals. In fact the ideas behind our choice of the subsets of path space and in the estimation of their probabilities comes partly from, by now, classical theory of large deviations for stochastic processes in the form initiated by Varadhan [55] (whose work has been generalized by Molčanov [38]) and developed by Ventcel and Freidlin [58, 59, 56] (see also [57]). Varadhan estimated the transition probability of diffusion processes: he seems to be the first to use a “geodesic idea” in this context. Ventcel and Freidlin's innovation is to express the probability that a path spend some time in a tube in terms of an action functional of the “center of the tube” [their ideas lead to extremizing problems of the type (2.30) below; see also Remark 4 after Proposition 2.5]. These asymptotics are accurate for small time. So we have to manufacture, in the same spirit, our own estimates relying on the very particularities of the situation we are dealing with (see for example Lemmas 2.2 and 2.3 below).

For a neat and self-contained exposition of the probability theory of large deviations the reader is referred to Azencott's lectures [8].

Moreover the occurrence of classical solutions or minimal action paths in the present kind of situation is common in the recent particle physics literature (see e.g. [33, 11]) in connection with tunneling problems: the fall off of wave functions can certainly be thought of as a tunneling problem since it asks for the value of φ in a classically forbidden region: the necessity for looking at $-V$ rather than V is well-known in such contexts.

For the N-body case, Agmon also found ϱ as a geodesic distance; again, his ϱ optimizes an inequality like (1.3), this time inequalities found initially by Deift et al. [17] (who did not find their systematic solution, but who often guessed the right answer), but also derived by Agmon. Agmon [1] also obtains pointwise bounds in this case.

To describe the function ϱ we need some multiparticle notations (that we will use freely in the sequel).

D denotes a generic partition of $\{1, \ldots, N\}$ into clusters and $\sum_{iDj}$ denotes the sum over all pairs $\{i,j\}$ in the same cluster. We deal with N ν-dimensional particles of masses $m_1, \ldots, m_N$ so we introduce the configuration space:

$$X = \left\{(x_1, \ldots, x_N) \in \mathbb{R}^{N\nu};\ \sum_{i=1}^{N} m_i x_i = 0\right\}$$

equipped with the norm:

$$\|x\| = \left(\sum_{i=1}^{N} m_i |x_i|^2\right)^{1/2}, \tag{1.7}$$

where $|\cdot|$ denotes the usual Euclidean norm in $\mathbb{R}^\nu$. H_0 will denote the free Hamiltonian for these N particles with center of mass motion removed viewed as an operator on $L^2(X)$ [note that $L^2(X)$ is understood with respect to the volume element corresponding to the metric (1.7) and that H_0 is nothing but minus a half the corresponding Laplace-Beltrami operator].

For each pair of indices $\{i,j\}$ we imagine a pair potential $V_{ij}(x_i - x_j)$ with

$$\lim_{|y| \to \infty} V_{ij}(y) = 0,$$

(and more precise hypotheses later). For each partition D we define:

$$H_D = H_0 + \sum_{iDj} V_{ij}(x_i - x_j)$$

which describe a system of non-interacting clusters and the threshold Σ_D by:

$$\Sigma_D = \inf \sigma(H_D),$$

where $\sigma(K)$ denotes the spectrum of the operator K.

Of course the full Hamiltonian of the system is defined on $L^2(X)$ by:

$$H = H_0 + \sum_{1 \leqq i < j \leqq N} V_{ij}(x_i - x_j).$$

For each $x = (x_1, \ldots, x_N) \in X$, we define $D(x)$ to be the partition obtained by lumping together those i and j with $x_i = x_j$, i.e. for all x with distinct x_i, $D(x)$ is the N cluster partition, but on various planes the codimension ν where some $x_i - x_j = 0$, $D(x)$ has a fewer number of clusters, etc.

Also note that:

$$\Sigma = \min_D \Sigma_D$$

is the infimum of the essential spectrum of H (we refer to [17] or [45] for kinematics in X). Agmon's formula for ϱ is:

$$\varrho(x)=\inf\left\{\int_0^t \sqrt{2(\Sigma_{D(\gamma(s))}-E)}\,\|\dot{\gamma}(s)\|\,ds;\ t\geqq 0,\ \gamma:[0,t]\to X,\ \gamma(0)=x,\ \gamma(t)=0\right\}. \tag{1.8}$$

Recall that, in this paper, all the trial paths we use are implicitly assumed to possess an almost everywhere derivative in L^1-sense. (Also we identify X and its tangent space.) The parameter E on which $\varrho(x)$ depends could be any number less than Σ. In fact, in the study of upper bounds ([1] and Sect. 5 below) E is any subcontinuum energy and in the study of lower bounds (which is our main concern) E is the ground state energy.

As in Sect. 2, there is a related formula which enters more naturally:

$$\varrho(x)=\inf\left\{\tfrac{1}{2}\int_0^t \|\dot{\gamma}(s)\|^2 ds+\int_0^t (\Sigma_{D(\gamma(s))}-E)ds;\ t\geqq 0,\ \gamma(0)=x,\ \gamma(t)=0\right\}. \tag{1.9}$$

Some of the geometry associated to these minimum problems is found in Appendix 3, where in particular, an explicit formula is given for $N=3$ and conjectured for general N. We give the lower bounds for $N=2,3$ in Sect. 3 and for general N in Sect. 4. In Sect. 5 we show how to use path integrals to get upper bounds in the N-body case.

We remark that correct lower bound for the (three body) ground state of Helium have been obtained previously by Hoffmann-Ostenhof [28, 5].

We emphasized above that all we deal with here is the leading behavior and the ground state. However, neither restriction is really rigid. Both the physics literature [14, 7] and the mathematics literature [41, 44] have amply demonstrated the possibility of doing asymptotics to very high order in path space and it should be possible to go to higher order here albeit with considerably greater effort; in certain situations, this has already been accomplished by Lieb and Simon [32].

The restriction to the ground state enters in the proof because in (1.5) one wants to know there are no cancellations possible between the region of path space estimated and other regions of path space; so long as φ is positive all contributions are positive. Of course if one is willing to make a detailed analysis of all of path space, this positivity is unnecessary. Even without such detailed analysis, one can handle certain other eigenfunctions as follows: suppose that φ is an eigenfunction which is positive in the region $\{|x|\geqq R\}$. Then, by using stopping time arguments, one can obtain a formula like (1.5) [but now t is the minimum of some fixed number t_0 and the first time s that $|x+b(s)|\leqq R$] with a nonnegative integrand in path space. Similarly, one can control asymptotics of φ in any region where it is known that the geodesic from x to 0 stays in a region where φ has fixed sign (e.g. this will be possible for the lowest eigenvalue of one dimensional fermions).

Of course for general eigenfunctions which typically have nodes running to infinity, one cannot hope to obtain pointwise lower bounds; the results of [9] suggest one should look for lower bounds on the average over geodesic sphere about $x=0$, i.e. over sets with $\varrho(x)=a$.

We should like to close this introduction with a discussion of the status of the earlier papers of the series since recent developments have made much of these papers obsolete.

Reference [46] dealt with two issues: results implying that $D(H^N)\subset L^\infty$ (for suitable N) and results on obtaining exponential fall off; substantial improvements, both in the hypotheses needed on the potential and on the value of N can be made with path integral methods: initial ideas are in Herbst and Sloan [22] with full developments independently due to the present authors [13, 49]. As we explain in Appendix 2, the best results on pointwise exponential fall off are easy to obtain via Harnack inequality methods.

Reference [47] dealt with fall off faster than any exponentials for situations where H has purely discrete spectrum. The only general improvement here is that hypotheses on V be bounded below are easy to remove with Harnack inequality methods (see Appendix 2).

Reference [48] dealt with several issues: the improved fall off for $V\to\infty$ is substantially improved by the "optional" upper bound of Agmon [1] (see also Appendix 1 and 2) and the related bound of Sect. 2 of this paper; results on the strict positivity of the ground state have been substantially improved by Carmona [13] (see also [30, 49, 25, 26]).

Most of [17] is not obsolete but can now have Agmon's optimal solution [1] of the inequalities of that paper; we also note that Agmon has an alternative method of proof leading to these equations.

2. The Case When $V(x)\to\infty$

Throughout this section V will be a continuous function obeying

$$\lim_{|x|\to\infty} V(x)=\infty \tag{2.1}$$

and

$$\forall x\in\mathbb{R}^\nu, \qquad V(x)\geqq 1 \tag{2.2}$$

(there is no real restriction since we can add a constant to V). φ will be a *positive* L^2 function obeying:

$$H\varphi=E\varphi, \tag{2.3}$$

with

$$H=-\tfrac{1}{2}\Delta+V. \tag{2.4}$$

At this point it is worthwhile noting that the assumption $\varphi\in L^2$ is much too restrictive for the proof of the main result of this section to work (nevertheless see Appendix 2). Indeed Theorem 2.1 below relies eventually on the fact that the function φ satisfies Feynman-Kac formula (1.5) and the latter can be derived provided φ satisfies (2.3) in the sense of distributions and does not increase too fast at infinity [for example if

$$\int \varphi(x)e^{-\varepsilon|x|^2}d^nx<+\infty$$

for all $\varepsilon > 0$]. Indeed, using a refined version of Ito's formula (see example [35]) it is easy to prove (1.5) with t replaced by the minimum of t and of the first exit time of a relatively compact open set, and this formula extends trivially to general time t because of the growth restriction on φ and because of (2.2).

Moreover we define:

$$W_{\pm}(x) = {}^{\sup}_{\inf}\{V(y); |x-y| \leqq 1\} \tag{2.5}$$

and

$$\varrho_{\pm}(x) = \inf\left\{\int_0^1 \sqrt{2W_{\pm}(\gamma(s))}|\dot{\gamma}(s)|ds; \gamma(0)=0, \gamma(1)=x\right\} \tag{2.6}$$

and

$$\varrho(x) = \inf\left\{\int_0^1 \sqrt{2V(\gamma(s))}\,|\dot{\gamma}(s)|ds; \gamma(0)=0, \gamma(1)=x\right\}. \tag{2.7}$$

In Appendix 2, we show that for any $\varepsilon > 0$, there is a constant C_ε with

$$\forall x \in \mathbb{R}^\nu, \quad |\varphi(x)| \leqq C_\varepsilon \exp[-(1-\varepsilon)\varrho_-(x)]. \tag{2.8}$$

Our main result in this section is:

Theorem 2.1. *For any $\varepsilon > 0$, there is a positive constant D_ε with:*

$$\forall x \in \mathbb{R}^\nu, \quad \varphi(x) \geqq D_\varepsilon \exp[-(1+\varepsilon)\varrho_+(x)]. \tag{2.9}$$

Remarks. 1. In (2.5), $|x-y| \leqq 1$ can be replaced by $|x-y| \leqq \delta$, for any $\delta > 0$ with no essential change.

2. Our proof actually yields something better than $\varepsilon\varrho_+(x)$, but it is still so far from the "next order" behavior, we have not bothered to give it explicitly.

3. Under fairly weak hypotheses, e.g. $\nabla V/V \to 0$ at infinity, one can show that $\varrho_+(x)/\varrho(x)$ and $\varrho_-(x)/\varrho(x)$ both go to one at infinity. In that case one can replace $\varrho_\pm$ in (2.8), (2.9) by ϱ and obtain:

$$\lim_{|x| \to \infty} - \frac{1}{\varrho(x)} \ln \varphi(x) = 1. \tag{2.10}$$

The proof of Theorem 2.1 will use Feynman-Kac formula (1.5). For a fixed trial function g with $g(0)=x$, $g(t)=0$, we will consider the contribution of paths with

$$|x + b(s) - g(s)| \leqq 1 \quad \text{for} \quad 0 \leqq s \leqq t.$$

The initial stages (Lemmas 2.2 and 2.3) will estimate the measure of this set of paths and will lead to the study of the variational problem associated to (1.6).

Lemma 2.2. *Let f be a fixed function with values in $\mathbb{R}^\nu$ with an almost everywhere L^2-derivative and with $f(0)=0$. Then:*

$$\mathbf{E}\{|b(s) - f(s)| \leqq 1, 0 \leqq s \leqq t\} \geqq e^{-\frac{1}{2}\int_0^t |\dot{f}(s)|^2 ds} \mathbf{E}\{|b(s)| \leqq 1, 0 \leqq s \leqq t\}, \tag{2.11}$$

where $\mathbf{E}$ is expectation with respect to ν-dimensional Brownian motion b starting at time $t=0$ from the origin, $\mathbf{E}\{A\} = \mathbf{E}\{\chi_A\}$ with χ_A the indicator function of the set A, and $|\dot{f}|^2$ means the square of the Euclidean norm of the vector $\dot{f}$.

Proof. Let Db denote the underlying measure whose expectation is $\mathbf{E}$ and let

$$A = \{|b(s)| \leqq 1, 0 \leqq s \leqq t\}.$$

The Cameron-Martin formula [36] says that:

$$\frac{D(b+f)}{Db} = \exp\left[-\tfrac{1}{2}\int_0^t |\dot{f}(s)|^2 ds - \int_0^t \dot{f}(s) \cdot db(s)\right]. \tag{2.12}$$

In (2.12) the left hand side is a Radon-Nikodym derivative and $\int - db(s)$ is an Ito-stochastic integral. By this formula:

$$\text{LHS of}\,(2.11) = \exp\left[-\tfrac{1}{2}\int_0^t |\dot{f}(s)|^2 ds\right] \mathbf{E}\left\{\exp\left[-\int_0^t \dot{f}(s) db(s)\right]\chi_A\right\}. \tag{2.13}$$

Now by Jensen's inequality for the measure $\frac{\chi_A}{\mathbf{E}\{\chi_A\}} Db$, we have that:

$$\mathbf{E}\left\{\exp\left[-\int_0^t \dot{f}(s) \cdot db(s)\right]\chi_A\right\} \geqq \mathbf{E}\{\chi_A\} \exp\left[-\mathbf{E}\left\{\chi_A \int_0^t \dot{f}(s) \cdot db(s)\right\}/\mathbf{E}\{\chi_A\}\right]. \tag{2.14}$$

Since A and Db are left invariant by the map $b \to -b$, and since $\int_0^t \dot{f}(s) \cdot db(s)$ is odd under this map, we have that:

$$\mathbf{E}\left\{\chi_A \int_0^t \dot{f}(s) \cdot db(s)\right\} = 0. \tag{2.15}$$

(2.13), (2.14), and (2.15) together imply (2.11). □

Remarks. 1. The same proof show that:

$$\mathbf{E}\{b - f \in A\} \geqq \exp\left[-\tfrac{1}{2}\int_0^t |\dot{f}(s)|^2 ds\right] \mathbf{E}\{A\}$$

for any set A invariant under $b \to -b$ and depending only on $b(s)$ for $0 \leqq s \leqq t$.

2. The combination of a Cameron-Martin formula followed by Jensen's inequality to get lower bounds is one that has been used in particular by Donsker and Varadhan in their celebrated work on asymptotics of functional integrals, see e.g. [18].

3. If one thinks of Db as $\exp\left[-\tfrac{1}{2}\int_0^t |\dot{b}(s)|^2 ds\right] \mathscr{D}b$ with $\mathscr{D}b$ a formally translation invariant measure, and of $\int_0^b \dot{f}(s) \cdot db(s)$ as $\int_0^t \dot{f}(s) \cdot \dot{b}(s) ds$, then (2.12) is formally obvious [the condition $f(0) = 0$ is needed since $\mathscr{D}b$ has a $\delta(b(0))$ corresponding to the $b(0) = 0$ boundary condition for Brownian motion]. For those unfamiliar or uncomfortable with stochastic integrals, one can prove (2.11) avoiding them by noting that:

$$\mathbf{E}\{|b(s) - f(s)| \leqq 1, 0 \leqq s \leqq t\} = \lim_{n\to\infty} \mathbf{E}\left\{\left|b\left(\frac{tj}{n}\right) - f\left(\frac{tj}{n}\right)\right| \leqq 1, j = 0, \ldots, n\right\}$$

by the continuity of paths and:

$$\mathbf{E}\left\{\left|b\left(\frac{tj}{n}\right)-f\left(\frac{tj}{n}\right)\right|\leqq 1, j=0,\ldots,n\right\}$$
$$\geqq \exp\left[-\tfrac{1}{2}\sum_{j=1}^{n}\left(\frac{t}{n}\right)^{-1}\left[f\left(\frac{jt}{n}\right)-f\left(\frac{(j-1)t}{n}\right)\right]^2\right]\mathbf{E}\left\{\left|b\left(\frac{tj}{n}\right)\right|\leqq 1, j=0,\ldots,n\right\}. \quad (2.16)$$

(2.11) follows as in the above proof but now (2.12) is replaced by a change of variable in a finite dimensional integral.

Lemma 2.3. *Let α be the lowest eigenvalue of the operator $H_D \equiv -\frac{1}{2}\Delta$ on $L^2(\{x;|x|\leqq 1\}, d^\nu x)$ with Dirichlet boundary condition. Then, for ν-dimensional Brownian motion and for all $t \geqq 0$, we have:*

$$\mathbf{E}\{|b(s)|\leqq 1; 0\leqq s\leqq t\}\geqq e^{-\alpha t}. \quad (2.17)$$

Proof. By a Feynman-Kac formula:

$$\text{LHS of (2.17)} = [e^{-tH_D}1](0), \quad (2.18)$$

where the 1 represents the function identically equal to one and the 0 means evaluated at the point zero. Let η be the (positive) eigenfunction of H_D with eigenvalue α *normalized* so that $\eta(0)=1$. Since $\eta(x)$ takes its maximum value at $x=0$ [10], $\eta\leqq 1$, so since e^{-tH_D} is positivity preserving

$$[e^{-tH_D}1](0)\geqq [e^{-tH_D}\eta](0)=e^{-t\alpha}\eta(0)=e^{-t\alpha}. \quad \square$$

Remarks. 1. (2.17) stills holds if $|b(s)|\leqq 1$ is replaced by $|b(s)|\leqq r$ and if $e^{-\alpha t}$ is replaced by $e^{-\alpha t/r^2}$.

2. Considering the simplicity of its proof, (2.17) is remarkably good. For example, the large t asymptotics of the left hand side of (2.17) is $ce^{-\alpha t}$ with $c=\int \eta(x)d^\nu x/\int \eta(x)^2 d^\nu x$. Thus, for $\nu=1$, $c=4/\pi$ and for $\nu=3$, $c=2$.

Putting together, the Feynman-Kac formula (1.5) and these last two lemmas, we see that:

Proposition 2.4. *Let $g=[0,T]\to\mathbb{R}^\nu$ be a C^1 function with $g(0)=x$ and $g(T)=0$. Then:*

$$\varphi(x)\geqq Ce^{(E-\alpha)T}e^{-\mathscr{A}_+(g)} \quad (2.19)$$

with:

$$C\equiv \inf_{|x|\leqq 1}\varphi(x)>0$$

and

$$\mathscr{A}_+(g)=\tfrac{1}{2}\int_0^t |\dot{g}(s)|^2 ds+\int_0^t W_+(g(s))ds. \quad (2.20)$$

Proof. By standard arguments [13, 49] φ is continuous, (1.5) holds for every $x\in\mathbb{R}^\nu$ and $t\geqq 0$ and C is strictly positive. The integrand in (1.5) is positive, so we can get a lower bound by taking a subset of paths. Take $t=T$ and those paths $b(s)$ with

$$\forall s\in[0,T], \quad |b(s)+x-g(s)|\leqq 1. \quad (2.21)$$

By the last two lemmas, the total measure of this set of paths is bounded from below by:

$$e^{-\alpha T} e^{-\frac{1}{2}\int_0^T |g(s)|^2 ds}.$$

Since (2.21) implies that:

$$\forall s \in [0, T], \qquad V(x + b(s)) \leqq W_+(g(s)),$$

the integrand for any such path is bounded from below by

$$C \exp\left[-\int_0^T W_+(g(s))ds\right]. \quad \square$$

Theorem 2.1 follows immediately from the last proposition and the following result which studies the function $\mathscr{A}_+$.

Proposition 2.5. *Let $\mathscr{A}_+$ be the functional defined by* (2.20) *and let:*

$$\mathscr{L}_+(\gamma) = \int_0^S \sqrt{2W_+(\gamma(s))}|\dot{\gamma}(s)|ds. \tag{2.22}$$

Then: (i) *There exist minimizing functions g and γ for $\mathscr{A}_+$ and $\mathscr{L}_+$ with the boundary conditions $g(0)=x$, $g(T)=0$, and $\gamma(0)=0$, $\gamma(s)=x$.*

(ii) *Any minimizing g for $\mathscr{A}_+$ yields, via $\gamma(s)=g(T-s)$, $0 \leqq s \leqq T=S$, a minimizing γ for $\mathscr{L}_+$, and in addition the minimum values are identical.*

(iii) *For each $x \in \mathbb{R}^\nu$, pick a minimizing g for $\mathscr{A}_+$ and let $T(x)$ be the corresponding value of T. Then:*

$$\lim_{|x| \to \infty} \frac{T(x)}{\varrho_+(x)} = 0. \tag{2.23}$$

Proof. (i) Existence of γ as minimizing γ for $\mathscr{L}_+$ is standard in differential geometry (see e.g. [42, 53]). Existence of a minimizing g is standard lower semi-continuity arguments (see e.g. [42]) if one notes that since $W_+ \geqq 1$, one can restrict attention to paths with an a priori upper bound on T (this is needed to assure compactness of the space of trial functions).

(ii) By the inequality:

$$ab \leqq \tfrac{1}{2}a^2 + \tfrac{1}{2}b^2, \tag{2.24}$$

we see that if γ_g is defined by $\gamma_g(s)=g(T-s)$, $0 \leqq s \leqq T=S$ then we have:

$$\mathscr{L}_+(\gamma_g) \leqq \mathscr{A}_+(g). \tag{2.25}$$

Since equality holds in (2.24) only if $a=b$, we have that equality holds in (2.25) if and only if

$$\forall s \in [0, T], \qquad |\dot{\gamma}(s)| = \sqrt{2W_+(\gamma(s))}. \tag{2.26}$$

Given any γ, we can always find a reparametrization $\tilde{\gamma}$ so that (2.26) holds for $\tilde{\gamma}$. Thus if $\tilde{g}$ is the corresponding g we have that:

$$\mathscr{A}_+(\tilde{g}) = \mathscr{L}_+(\tilde{\gamma}) = \mathscr{L}_+(\gamma)$$

since $\mathscr{L}_+$ is invariant under reparametrization. Equality of the minima is now obvious, and moreover by (2.26) and (2.25) any minimizing g obeys

$$\forall s \in [0, T], \quad |\dot{g}(s)| = \sqrt{2W_+(g(s))}\,. \tag{2.27}$$

(iii) By (2.27), if g is any minimizing g, then

$$\varrho_+(x) = 2 \int_0^{T(x)} W_+(g(s))ds\,. \tag{2.28}$$

Since $W_+ \geqq 1$, we see that:

$$T(x) \leqq \tfrac{1}{2}\varrho_+(x)\,. \tag{2.29}$$

Fix some $R_0 > 0$ and let $a(R_0) = \min_{|x| \geqq R_0} W_+(x)$. If $|x| > R_0$, let s_0 be the first time that $|g(s_0)| = R_0$. Then $s \to g(s+s_0)$ on $[0, T(x) - s_0]$ is a minimizing path for the problem with initial point $g(s_0)$, so by (2.29) we have:

$$T(x) - s_0 \leqq \tfrac{1}{2} \sup_{|y| = R_0} \varrho_+(y)\,.$$

Since $|g(s)| \geqq R_0$ for $s \in [0, s_0]$, we have that

$$\varrho_+(x) \geqq 2 s_0 a(R_0)$$

by (2.28) and the definition of $a(R_0)$. Thus

$$T(x) \leqq [2a(R_0)]^{-1} \varrho_+(x) + \tfrac{1}{2} \sup_{|y| = R_0} \varrho_+(y)\,.$$

From this, (2.23) follows immediately. □

Remarks. 1. Roughly speaking if V is reasonably behaved at infinity, $\dfrac{T(x)}{\varrho(x)} \sim \dfrac{1}{V(x)}$.

2. The equality of the minima of $\mathscr{A}_+$ and $\mathscr{L}_+$ is even easier than the more usual [42] equality of the minimum of $\mathscr{L}_+$ and

$$\sqrt{\xi_+(\gamma)} = \left[\int_0^1 2W_+(\gamma(s))|\dot{\gamma}(s)|^2 ds\right]^{1/2} \tag{2.30}$$

except that the numerical inequality (2.23) that we use is replaced by the Schwarz inequality on integrals in the usual case.

3. There is an illuminating alternative way of deriving (2.27). By rescaling $g(s)$ to $g(\lambda^{-1}s)$ one sees that for the minimizing g we have that:

$$\tfrac{1}{2}\int_0^1 |\dot{g}(s)|^2 ds = \int_0^1 W_+(g(s))ds\,. \tag{2.31}$$

Euler-Lagrange's equation associated to $\mathscr{A}_+$ (for fixed T) is just the classical equation:

$$\ddot{g}(s) = \nabla W_+(g(s))$$

(note: not $-\nabla W_+$) for which the conserved energy is:

$$\tfrac{1}{2}|\dot{g}(s)|^2 - W_+(g(s)) = C\,,$$

but by (2.31), $C = 0$.

4. Let us give another reason why the reparametrization of the paths is natural. The eigenvalue problem (2.3) can be rewritten in the form

$$-\frac{1}{2V(x)}\Delta\varphi(x)+U(x)\varphi(x)=0$$

with $U(x)=1-\frac{E}{V(x)}$. Using Feynman-Kac formula we have that:

$$\varphi(x)=\mathbf{E}_x\left\{\varphi(X_t)e^{-\int_0^t U(X_s)ds}\right\}, \tag{2.32}$$

where X_t denotes the diffusion process governed by the operator $-\frac{1}{2V(x)}\Delta$ and $\mathbf{E}_x$ denotes expectation over paths starting at x at time $t=0$. This process is in fact a Brownian motion process up to a time change. Namely, if we set

$$a_t=\int_0^t V(x+b(s))ds$$

and τ_t for its reciprocal function, that (2.32) can be rewritten in the form:

$$\varphi(x)=\mathbf{E}\left\{\varphi(x+b(\tau_t))e^{-\int_0^t U(x+b(\tau_s))ds}\right\}$$

and if we use Ventcel-Freidlin type estimates, we are automatically conducted (because of the reparametrization of the paths via τ_t) to the study of the function $\sqrt{\xi_t}$.

The last two propositions immediately imply Theorem 2.1 as already remarked.

We close this section with several comments.

In obtaining a bound like

$$\forall x\in\mathbb{R}^\nu, \qquad \varphi(x)\geqq C_3\exp[-(1+\varepsilon)\varrho(x)],$$

the $\varepsilon\varrho(x)$ is needed to accomodate two facts: the change from ϱ_+ to ϱ which is typically of order $|x|^{-1}\varrho(x)$, and the $T(x)$ which is typically of order $V(x)^{-1}\varrho(x)$. Thus, improved lower bounds are implicit in the above.

Next, let us be more explicit about the argument to accommodate eigenfunctions φ with $\varphi(x)>0$ for $|x|\geqq R$. Begin by noting that for $|x|>R$

$$\varphi(x)=\mathbf{E}\left\{\varphi(x+b(T))e^{\int_0^T [E-V(x+b(s))]ds}\right\},$$

where

$$T=T(b)\equiv\min(t_0,\inf\{s>0;|x+b(s)|=R\}).$$

Now fix $|x|>R+2$, take the geodesic from x to 0 and run it to the earliest time t_0 for which $|g(s)|=R+1$. Take paths b with $|x+b(s)-g(s)|\leqq 1$ for all $s\in[0,t_0]$, where g is this geodesic.

For such path $T(b)=t_0$ and we can argue as above using:

$$\varphi(x+b(T))\geqq\inf_{R+1\leqq|y|\leqq R+3}\varphi(y)>0$$

for such b's.

Next we note that if $\nu=1$, the geodesic is just a straight line and so

$$\varrho(x)=\int_0^{|x|}\sqrt{2V(y)}\,dy$$

as familiar with W.K.B. theory.

Finally we remark on an example of Agmon [2]; consider a "wavy" unbounded region Ω, for example the planar region:

$$\Omega=\{(x,y)\in\mathbb{R}^2;|y-x^2\sin x|<|x|\}.$$

Let $2H_D$ be the Dirichlet Laplacian for $L^2(\Omega)$ and let $V\in C_0^\infty$ be such that H_D+V has a square integrable ground state φ. Suppose that:

$$(H_D+V)\varphi=E\varphi$$

with $E=-\frac{1}{2}k^2$. One might think that $\varphi(x)\sim e^{-k|x|}$, which is the case if Ω is all of $\mathbb{R}^2$. What happens now is that by his method one can prove a better bound, namely

$$\varphi(x)\leqq c_1e^{-k\varrho(x)}$$

with $\varrho(x)$ the geodesic distance from x to the origin with the usual Euclidean metric, but with the restriction that the curve stays inside Ω. Thus, in the example above, if we take $x_n=(n\pi,0)$, $\varrho(x_n)\sim cn^2$ not n. By going through the above proof get that for any curve g such that g lies in:

$$\Omega^\delta=\{x;\{y;|y-x|\leqq\delta\}\subset\Omega\}$$

one has:

$$\varphi(x)\geqq C\exp\left[(E-\delta^{-2}\alpha)t-\int_0^t|g(s)|^2ds\right]$$

which leads to the lower bound:

$$\varphi(x)\geqq C_\delta\exp[-k_\delta\varrho_\delta(x)]$$

with $\varrho_\delta(x)$ the geodesic distance within Ω^δ and k_δ given by

$$-\tfrac{1}{2}k_\delta^2=E-\delta^{-2}\alpha.$$

3. Lower Bounds, some Special N-Body Systems

In this section we describe the proof of the N-body lower bound in two "warm up" cases which will illustrate the main ideas: the case $N=2$ and the special $N=3$ case associated with the ground state of the Helium atom (in the purely Coulomb, infinite nuclear mass approximations).

First we begin by some notations and preliminary results needed in the sequel. In the next sections, we consider N particles with masses $m_1,\dots,m_N$ in ν-dimensions. In order to use path integral techniques we introduce the X-valued Brownian motion $\{b(t);t\geqq0\}$ canonically associated with the Euclidean structure of X. We call this process the *mass weighted Brownian motion.* The point is that if H_0 is the free Hamiltonian with center of mass motion removed, then for $\psi\in L^2(X)$,

$t>0$, and $x\in X$ we have:

$$[e^{-tH_0}\psi](x)=\mathbf{E}\{\psi(x+b(t))\}$$

and Lemma 2.2 now take form:

$$\mathbf{E}[b-f\in A\}\geqq \exp\left[-\tfrac{1}{2}\int_0^t \|\dot{f}(s)\|^2 ds\right]\mathbf{E}\{b\in A\}, \tag{3.1}$$

where A is a set of X-valued paths on $[0,t]$ invariant under the map $b\to -b$, f is a X-valued function with $f(0)=0$ and the norm $\|\cdot\|$ is that of (1.7). Moreover, under the usual assumptions on the potentials V_{ij}, we have the general Feynman-Kac formula for the full N-body Hamiltonian H:

$$[e^{-tH}\psi](x)=\mathbf{E}\left\{\psi(x+b(t))\exp\left[-\int_0^t \sum_{1\leqq i<j\leqq N} V_{ij}(x_i+b_i(s)-x_j-b_j(s))ds\right]\right\}$$

for all $\psi\in L^2(X)$, $t>0$ and $x\in X$, where $b_1(\cdot),\dots,b_N(\cdot)$ denote the components of $b(\cdot)$ when X is viewed as a subset of $\mathbb{R}^{N\nu}$. The reader should keep in mind the fact that the components $b_1(\cdot),\dots,b_N(\cdot)$ of the process $b(\cdot)$ *are not independent*; indeed with probability one we have that for all $t>0$

$$\sum_{i=1}^N m_i b_i(t)=0,$$

even though, for *each fixed* i, the process $b_i(t)$ is usual ν-dimensional Brownian motion and consequently is of the form $b_i(t)=\{b_{i,\alpha}(t);\alpha=1,\dots,\nu\}$ where the $b_{i,\alpha}(t)$ are ν independent one dimensional Brownian motions.

In fact the mass weighted Brownian motion can be thought of as the $N\nu$ dimensional mean zero Gaussian process $\{b_{i,\alpha}(t);\ i=1,\dots,N,\ \alpha=1,\dots,\nu,\ t\geqq 0\}$ whose covariance is given by:

$$\mathbf{E}\{b_{i,\alpha}(t)b_{j,\beta}(s)\}=A_{ij}\delta_{\alpha,\beta}\min(s,t)$$

with

$$A_{ij}=-M^{-1}+m_i^{-1}\delta_{ij}\qquad i,j=1,\dots,N$$

and

$$M=\sum_{i=1}^N m_i.$$

Second, we prove a little lemma that says that (even in the general N-body case) we can essentially restrict attention to potentials in C_0^∞!

Lemma 3.1. *Let φ be the ground state of an N-body Hamiltonian H with potentials V_{ij} in $L^p(\mathbb{R}^\nu)+L^\infty_\varepsilon(\mathbb{R}^\nu)$ for some $p>\nu/2$. Then, for any $\varepsilon'>0$, $\delta>0$, and $\mu>0$, there exist constants $C>0$, $q>1$ and potentials $W_{ij}\in C_0^\infty$ so that:*

$$\text{(i)}\quad \varphi(x)\geqq Ce^{(E-\mu)t}\mathbf{E}\left\{\varphi(x+b(t))^{1/q}\exp\left[-\int_0^t W(x+b(s))ds\right]\right\}^q \tag{3.2}$$

for all $t>0$ *and* $x\in X$, *where* $W(x)=\sum_{1\leqq i<j\leqq N} W_{ij}(x_i-x_j)$ *and* $\mathbf{E}$ *denotes the expectation with respect to mass weighted Brownian motion.*

(ii) $q\leqq 1+\delta$.

(iii) *For every partition D we have:*

$$|\Sigma'_D-\Sigma_D|\leqq\varepsilon',$$

where Σ_D *(respectively* Σ'_D*) is the threshold given by the infimum of the spectrum of* $H_D\left(\text{respectively } H_0+\sum_{iDj} W_{ij}\right)$.

Proof. Let $V=q(W+Y)$ where $1<q<1+\delta$, W_{ij} and Y_{ij} are functions of x_i-x_j, and $W=\sum_{i<j} W_{ij}$ and $Y=\sum_{i<j} Y_{ij}$. Then by Hölder's inequality we have:

$$\mathbf{E}\{\varphi^{1/q}e^{-\int(W-q^{-1}E)}\}\leqq\mathbf{E}\{\varphi e^{-\int V-E}\}^{1/q}\mathbf{E}\{e^{q'\int Y}\}^{1/q'}$$

with q' the conjugate exponent of q. Thus, using Feynman-Kac formula we have:

$$\varphi(x)\geqq f(t)\mathbf{E}\left\{\varphi(x+b(t))^{1/q}\exp\left[-\int_0^t(W(x+b(s))-q^{-1}E)ds\right]\right\}^q \tag{3.3}$$

where:

$$f(t)=\left[\sup_{x\in\mathbb{R}^{N\nu}}\mathbf{E}\left\{e^{q\int_0^t Y(x+b(s))ds}\right\}\right]^{-q/q'}.$$

For each pair $i<j$, let $\{W_{ij}^{(n)};n\geqq 1\}$ be a sequence in C_0^∞ so that:

$$Y_{ij}^{(n)}\equiv q^{-1}V_{ij}-W_{ij}^{(n)}\xrightarrow[n\to\infty]{}0\quad\text{in }(L^p+L_\varepsilon^\infty\text{-norm}).$$

For each partition D and $n\geqq 1$, let $\Sigma_D^{(n)}$ be the threshold corresponding to the infinum of the spectrum of $H_0+\sum_{iDj}W_{ij}^{(n)}$. By picking q close enough to 1 and then n large enough (how large depending only on ε and q) we can be sure that:

$$|\Sigma_D-\Sigma_D^{(n)}|<\varepsilon'$$

for all partitions D. Increasing n if necessary, the $(L^p+L_\varepsilon^\infty)$-norm of $Y_{ij}^{(n)}$ can be made arbitrarily small so that, by the basic estimation of:

$$\|e^{-t(H_0+qY)}\|_{\infty,\infty}=\sup_{x\in\mathbb{R}^{N\nu}}\mathbf{E}\left\{e^{\int_0^t qY(x+b(s))ds}\right\}$$

in [13, 30, 48], we can be sure that $f(t)$ (with Y replaced by $Y^{(n)}$) satisfies

$$f(t)^{-1}\leqq C^{-1}e^{\mu t},$$

which, together with (3.3) gives (3.2). □

With this lemma, the lower bound in case $N=2$ is easy (it is also easy by other methods).

Theorem 3.2. *Let* $V\in L^p(\mathbb{R}^\nu)+L_\varepsilon^\infty(\mathbb{R}^\nu)$ *with* $p>\nu/2$, *let* $H=-\frac{1}{2}\Delta+V$ *on* $L^2(\mathbb{R}^\nu)$ *and let us assume that* $\varphi\in L^2(\mathbb{R}^\nu)$ *is nonnegative and satisfies:*

$$H\varphi=-\tfrac{1}{2}k^2\varphi$$

for some $k>0$. *Then, for any* $\varepsilon>0$ *there exists a constant* $C_\varepsilon>0$ *such that:*

$$\forall x\in\mathbb{R}^\nu, \quad \varphi(x)\geqq C_\varepsilon \exp[-(1+\varepsilon)k|x|].$$

Proof. Choose W in C_0^∞ so that (3.2) holds with $\mu=\frac{1}{3}\varepsilon k^2$, $\delta=\frac{2}{3}\varepsilon$ and any $\varepsilon'>0$. Let us assume that $R_0>0$ is such that $\{x\in\mathbb{R}^\nu; |x|\leqq R_0\}$ contains the support of W, and let us fix $R>0$. Given $x\in\mathbb{R}^\nu$ with $|x|>R+R_0$, let g be the linear path of constant velocity, defined on $[0,t]$ and such that $g(0)=x$ and $g(t)=(R+R_0)x/|x|$. In (3.2) take the contribution of those paths b such that:

$$\forall s\in[0,t], \quad |x+b(s)-g(s)|\leqq R. \tag{3.4}$$

For such paths, $W(x+b(s))=0$ for all s in $[0,t]$ so that:

$$\begin{aligned}\varphi(x)&\geqq Ce^{-(\frac{1}{2}k^2+\mu)t}(\inf_{|Y|\geqq R_0+2R}\varphi(Y))\mathbf{E}\{|x+b(s)-g(s)|\leqq R; 0\leqq s\leqq t\}^q\\ &\geqq C(\inf_{|Y|\leqq R_0+2R}\varphi(Y))\exp\left[-\left(\tfrac{1}{2}k^2+\mu+\frac{q}{2}v^2+q\alpha R^{-2}\right)t\right],\end{aligned}$$

where $v=|x|(1-(R+R_0)|x|^{-1})t^{-1}\leqq|x|t^{-1}$ and α has been defined in Lemma 2.3. Now if we pick $t=|x|k^{-1}$ and R so that $q\alpha R^{-2}=\frac{1}{3}\varepsilon k$, we find that

$$\varphi(x)\geqq C_\varepsilon\exp[-(1+\varepsilon)k|x|]$$

with:

$$C_\varepsilon=C\inf_{|Y|\leqq R_0+2R}\varphi(Y)>0. \quad \square$$

Now let us consider the operator

$$H=-\tfrac{1}{2}\Delta_1-\tfrac{1}{2}\Delta_2+U(x_1)+U(x_2)+W(x_{12}) \tag{3.5}$$

on $L^2(\mathbb{R}^6)$ where Δ_i denotes Laplacian on $L^2(\mathbb{R}^3)$ for the variable $x_i\in\mathbb{R}^3$, $i=1,2$, and where $x_{12}=x_1-x_2$. We will write $x=(x_1,x_2)\in\mathbb{R}^6$ and $H=-\frac{1}{2}\Delta+V(x)$ with $V(x)=U(x_1)+U(x_2)+W(x_{12})$. Note that in the present situation $X=\mathbb{R}^6$ with its usual Euclidean structure so that $\|\cdot\|$ is the usual Euclidean norm $|\cdot|$ and the mass weighted Brownian motion $b(t)=(b_1(t),b_2(t))$ is the usual 6-dimensional Brownian motion. We suppose $U\leqq 0$, $W\geqq 0$, spherically symmetric, continuous and going to zero at infinity and let $E=-(\varepsilon_1+\varepsilon_2)$ be the ground state energy of H and $-\varepsilon_2$ be the ground state energy of $-\frac{1}{2}\Delta_1+U(x_1)$. Of necessity:

$$\varepsilon_1<\varepsilon_2 \tag{3.6}$$

since $W\geqq 0$. We want to prove that for each $\varepsilon>0$ there is a constant $C_\varepsilon>0$ for which:

$$\forall x\in\mathbb{R}^6, \quad \varphi(x)\geqq C_\varepsilon\exp[-(1+\varepsilon)\varrho(x)] \tag{3.7}$$

with:

$$\varrho(x)\equiv\sqrt{2\varepsilon_1}\max(|x_1|,|x_2|)+\sqrt{2\varepsilon_2}\min(|x_1|,|x_2|). \tag{3.8}$$

We show in Appendix 3 that ϱ is the Agmon metric for this case.

The point is that if we look at the contribution of the set of paths which satisfy (3.4), their measure will give us a factor of $\exp\left[-\frac{1}{2}\int_0^t|\dot{g}(s)|^2ds\right]$ as usual. When R is large, but still small compared to $|x|$, we can drop all interactions except those that act for times proportional to $|x|$, i.e. keep only the interactions $\sum_{iD(g(s))j} V_{ij}$, and the allowed large R Brownian fluctuations will produce a time ordered exponential $T(\exp[-H^R_{D(g(s))}])$ where the superscript R indicates a Dirichlet boundary condition on the ball of radius R. This exponential should look like $\exp\left[-\int_0^t \Sigma_{D(g(s))}ds\right]$ so that the variational principle will enter. Having given the heuristic argument, we present the details.

Without any loss of generality we can assume $|x_1| \geqq |x_2|$. The minimizing path for the variational principle (1.9) is:

$$[0, t] \ni s \to g(s) = (g_1(s), g_2(s)) \in \mathbb{R}^6,$$

where $t = |x_1|/\sqrt{2\varepsilon_1}$ and:

$$g_1(s) = x_1(1 - s|x_1|^{-1}\sqrt{2\varepsilon_1}) \qquad 0 \leqq s \leqq t$$

and:

$$g_2(s) = \begin{cases} x_2(1 - s|x_2|^{-1}\sqrt{2\varepsilon_2}) & 0 \leqq s \leqq t' \\ 0 & t' \leqq s \leqq t, \end{cases}$$

where $t' = |x_2|/\sqrt{2\varepsilon_2}$. Notice that since $|x_2| \leqq |x_1|$ and $\varepsilon_2 > \varepsilon_1$, we have that $t' \leqq t$. Notice also that:

$$\Sigma_{D(g(s))} = \begin{cases} 0 & \text{if } 0 \leqq s \leqq t' \\ -\varepsilon_2 & \text{if } t' \leqq s \leqq t \end{cases}$$

so that:

$$\begin{aligned} \int_0^t (E - \Sigma_{D(g(s))})ds &= t'(\varepsilon_1 + \varepsilon_2) + (t - t')\varepsilon_1 \\ &= \varepsilon_2 t' + \varepsilon_1 t \\ &= \tfrac{1}{2}\varrho(x), \end{aligned} \tag{3.9a}$$

and:

$$\begin{aligned} \tfrac{1}{2}\int_0^t |\dot{g}(s)|^2 ds &= \tfrac{1}{2}[t(2\varepsilon_1) + t'(2\varepsilon_2)] \\ &= \tfrac{1}{2}\varrho(x). \end{aligned} \tag{3.9b}$$

The total time t involved in this path grows at the same rate as $\varrho(x)$ (i.e. $t/\varrho(x)$ is bounded above and below) so we need only prove that:

$$e^{ET}\mathbf{E}\left\{e^{-\int_0^t V(x+b(s))ds}\varphi(x+b(t))^{1/p}\right\}^p \geqq C_\varepsilon e^{-(1+\frac{1}{2}\varepsilon)\varrho(x)}, \tag{3.10}$$

where V is obtained from spherically symmetric potentials U and W in C_0^∞, with identical thresholds since the $\frac{1}{2}\varepsilon\varrho(x)$ can be used to accommodate the changes in thresholds, the factor of $e^{-\mu t}$, and the changes from arbitrary U, W to C_0^∞ potentials.

Let R_0 be such that:

$$|Y|>R_0 \Rightarrow U(Y)=0 \quad \text{and} \quad W(Y)=0,$$

and let:

$$k=\max(\|U\|_\infty, \|W\|_\infty).$$

We will look at paths $b(\cdot)$ satisfying

$$|x+b(s)-g(s)| \leqq R, \qquad 0 \leqq s \leqq t,$$

where R is a number to be adjusted later on. For any such path we claim that:

$$-\int_0^t V(x+b(s))ds \geqq -\int_{t'}^t U(x_2+b_2(s))ds - C_0, \tag{3.11}$$

where C_0 is a *fixed* constant *independent* of x (but depending on R, R_0 and K). For the total time τ' during $[0,t']$ that either $|g_1(s)|<R_0+R$ or $|g_2(s)|<R+R_0$ or $|g_1(s)-g_2(s)|<R_0+2R$ is bounded independently of $|x|$, and similarly for the total time τ during $[t',t]$ for which $|g_1(s)|<R_0+2R$. So one can take C_0 in (3.11) to be $3(\tau'+\tau)K$.

Using the translation formula (3.1) and (3.11) one finds that:

$$[\text{L.H.S. of (3.10)}] \geqq C \exp\left[-\tfrac{1}{2}\int_0^t |\dot{g}(s)|^2 ds\right] e^{Et} \mathbf{E}\left\{\exp\left[-\int_{t'}^t U(b_2(s))ds\right]; A\right\}, \tag{3.12}$$

where C has a factor of $e^{-C_0 P}$ and of $\inf_{|y| \leqq R} \varphi(y)$, where:

$$A=\{b=(b_1,b_2);\ |b_1(s)|^2+|b_2(s)|^2 \leqq R^2,\ t' \leqq s \leqq t\},$$

and where $\mathbf{E}\{f;A\}$ stands for $\mathbf{E}\{f\chi_A\}$ with χ_A the indicator function of the set A.

Let H_0^R be $-\frac{1}{2}\Delta_1-\frac{1}{2}\Delta_2$ with Dirichlet boundary condition on the sphere of radius R and let $H_1^R=H_0^R+U(r_2)$. Then the expectation in the right hand side of (3.12) is just:

$$[e^{-t'H_0^R} e^{-(t-t')H_1^R} \chi_R](0) \tag{3.13}$$

with χ_R the indicator function of the ball $\{x \in \mathbb{R}^6; |x| \leqq R\}$. Let $\alpha_0^{R/2}$ and α_1^R be the lowest eigenvalues of $H_0^{R/2}$ and H_1^R, and let $\eta_0^{R/2}$ and η_1^R be the corresponding ground states. Then:

$$\begin{aligned} e^{-(t-t')H_1^R}\chi_R &\geqq C_1[e^{-(t-t')H_1^R}\eta_1^R] \\ &= C_1 e^{-(t-t')\alpha_1^R}\eta_1^R \\ &\geqq C_1 C_2 e^{-(t-t')\alpha_1^R}\eta_0^{R/2}, \end{aligned}$$

where

$$C_1=\|\eta_1^R\|_\infty^{-1} \quad \text{and} \quad C_2=\|\eta_0^{R/2}/\eta_1^R\|_\infty^{-1}.$$

Thus (3.13) is bounded from below by a constant times:

$$\exp[-(\alpha_0^{R/2}t'+\alpha_1^R(t-t'))].$$

By choosing R sufficiently large we can be sure that, up to errors which are small of the order of t,

$$\alpha_0^{R/2}t' + \alpha_1^R(t-t') \cong \tfrac{1}{2}\varrho(x).$$

Putting this together with (3.10), (3.12), and (3.9a, b) we obtain (3.7) as desired.

In the above, when we used (3.1), we actually used it in a slightly extended form; namely, rather than (3.1) we used:

$$\mathbf{E}\{G_f; A_f\} \geqq \exp\left[-\tfrac{1}{2}\int_0^t |\dot{f}(s)|^2 ds\right] \mathbf{E}\{G; A\}, \tag{3.1'}$$

where:

$$A_f = \{b; b-f \in A\} \quad \text{and} \quad G_f(b) = G(b-f)$$

with G and even positive function of b. It was because of this evenness requirement that we careful to require spherically symmetric potentials since, in the above:

$$G(b) = \exp\left[-\int_{t'}^t U(b_2(s))ds\right].$$

Having made this remark, we want to show that one can still get a lower bound if U is not even. The point is simple: in using Jensen's inequality, what enters is:

$$\mathbf{E}\left\{G(b)\int_0^t \dot{g}\cdot db; A\right\} / \mathbf{E}\{G(b); A\}, \tag{3.14}$$

where A is the set of paths defined by:

$$A = \{b = (b_1, b_2); |b_1(s)|^2 + |b_2(s)|^2 \leqq R^2, 0 \leqq s \leqq t\}.$$

(3.14) is definitely *not* zero in general if U is not even, but since $\dot{g}$ is piecewise constant, we have:

$$\begin{aligned}\int_0^t \dot{g}(s)\cdot db(s) &= \dot{g}\left(\frac{t'}{2}\right)\int_0^{t'} db(s) + \dot{g}\left(\frac{t+t'}{2}\right)\int_{t'}^t db(s)\\ &= \dot{g}\left(\frac{t'}{2}\right)\cdot b(t') + \dot{g}\left(\frac{t+t'}{2}\right)\cdot [b(t) - b(t')].\end{aligned}$$

Since b is bounded on the set A, we see that:

$$|(3.14)| \leqq R\left[\left|\dot{g}\left(\frac{t'}{2}\right)\right| + 2\left|\dot{g}\left(\frac{t+t'}{2}\right)\right|\right], \tag{3.15}$$

and thus one can still get a lower bound [although, since R may have to be chosen very large, the use of (3.15) will lead to obscenely small constants; but, of course the arguments already given will lead to pretty bad constants since $\inf_{|y| \leqq R_0 + 2R} \varphi(y)$ is also exponentially small as $R \to \infty$].

4. Lower Bounds for General N-Body Ground States

In this section, we want to sketch the proof of the following result, which, together with Theorem 2.1, is one of the two principal results of the paper:

Theorem 4.1. *Let $H\varphi = E\varphi$ where H is an N-body Schrödinger Hamiltonian with two body potentials V_{ij} in $L^p + L^\infty_\varepsilon$ with $p > \nu/2$. Suppose $\varphi \in L^2(X)$ and $\varphi \geqq 0$. Then, for any $\varepsilon > 0$, there is a C_ε with:*

$$\forall x \in X, \quad \varphi(x) \geqq C_\varepsilon \exp[-(1+\varepsilon)\varrho(x)], \tag{4.1}$$

where ϱ is the Agmon metric. In particular, given the upper bound of Agmon [1] *(see Appendix 1), we have:*

$$\lim_{\substack{|x|\to\infty \\ x/|x|\to\hat{e}}} -\frac{1}{|x|}\ln\varphi(x) = \varrho(\hat{e}).$$

The initial steps in the proof (Lemmas 4.2, 4.3) will show that it suffices to prove (4.1) as $x \to \infty$ inside a small tube about any fixed direction with a constant C which a priori could be direction dependent (let us remark that by using a Harnack inequality [20, 54], one can even reduce it to a bound in each fixed direction but in the proof it is not hard to directly obtain the tube about each direction).

Lemma 4.2. *Let $\hat{e}$ be a fixed unit vector. Suppose that for all x with $\|x - \|x\|\hat{e}\| \leqq 1$ we have:*

$$\varphi(x) \geqq C \exp[-(1+\varepsilon)\|x\|\varrho(\hat{e})]. \tag{4.2}$$

Then there exist $D > 0$ and $\delta > 0$ such that:

$$\varphi(x) \geqq D \exp[-(1+2\varepsilon)\varrho(x)] \tag{4.3}$$

for all x with $\| \|x\|^{-1}x - \hat{e}\| < \delta$.

Proof. Let d denote the full Agmon metric so that $\varrho(x) = d(x, 0)$. Clearly:

$$\sqrt{-2(E-\Sigma)}\,\|x-y\| \leqq d(x,y) \leqq \sqrt{-2E}\,\|x-y\|$$

with $\|\cdot\|$ the mass weighted norm (1.7). Note that $\varphi \geqq 0$ implies that E is the ground state energy and consequently $E < \Sigma$. Now since:

$$|\varrho(x) - \varrho(y)| \leqq d(x,y)$$

we see that ϱ is continuous on the unit sphere and thus we need only prove (4.3) with $(1+2\varepsilon)\varrho(x)$ replaced by $(1+\varepsilon)\|x\|\varrho(\hat{e}) + \varepsilon'\|x\|$ for small ε'.

By the Schwarz inequality and Feynman-Kac formula, for any t and x:

$$\begin{aligned}\mathbf{E}\{\varphi(x+b(t))^{1/2}\}^2 &\leqq \mathbf{E}\left\{\varphi(x+b(t))e^{-\int_0^t (V(x+b(s))-E)ds}\right\}\mathbf{E}\left\{e^{\int_0^t (V(x+b(s))-E)ds}\right\} \\ &\leqq C'\varphi(x)e^{At},\end{aligned} \tag{4.4}$$

where we used the estimates of [13, 49] to bound $\mathbf{E}\left\{e^{\int_0^t (V(x+b(s))-E)ds}\right\}$. In (4.4) C' and A are fixed constants. Now, fix x with $\| \|x\|^{-1}x - \hat{e}\| < \delta$, suppose that (4.2) holds for y with $\|y - \|y\|\hat{e}\| \leqq 1$, and take $t = \mu\|x\|$ in (4.4) to find:

$$\varphi(x) \geqq C'^{-1}e^{-A\mu\|x\|}Ce^{-(1+\varepsilon)\|x\|\varrho(\hat{e})}C''\|x\|^{-(N-1)\nu/2}e^{-\delta^2|x|^2/2\mu|x|}.$$

This follows by looking at the contribution of those points y with $y = x + b(t)$ and $\|y - \|y\|\hat{e}\| \leqq 1$ [exploiting the explicit distribution of $b(t)$ and the fact that

$\|x-y\| \leqq \delta\|x\|$ for such y]. Taking first μ small and then δ small compared to μ, we obtain the required estimate. □

Lemma 4.3. *If for each* ε *and* $\hat{e}$ *there exists a* C *so that* (4.2) *holds for all* x *with* $\|x-\|x\|\hat{e}\|<1$, *then for all* $\varepsilon>0$ *there is a* C_ε *with* (4.1) *holding.*

Proof. This follows from Lemma 4.2 and an easy compactness argument. □

The reason we needed the above preliminaries is the following: we know almost nothing about the detailed structure of Agmon geodesics for $N \geqq 4$; in particular, we don't know that there aren't infinitely many linear segments (although we conjecture there are at most N). Thus, the natural estimates lead to constants which a priori depend on $x/\|x\|$. The above "compactness" argument then allows us to get a uniform constant.

Proof of Theorem 4.1. By the last two lemmas, we fix a unit vector $\hat{e}$ in X and study a neighbourhood of $\{\lambda\hat{e}; \lambda \in \mathbb{R}\}$.

Step 1. Picking an approximate geodesic

We first pick a function g_0 on $[0, T]$ with $g_0(0)=\hat{e}$, $g_0(T)=0$ and so that there exists $0=t_0<t_1<\ldots<t_k=T$ with $\dot{g}_0(s)$ and $D(g_0(s))$ constant on each interval (t_i, t_{i+1}) [Note: if a linear segment crosses a plane where $D(g_0(s))$ changes, then we consider it as two segments] and finally so that:

$$\tfrac{1}{2}\int_0^T \|\dot{g}_0(s)\|^2 ds + \int_0^T (\Sigma_{D(g_0(s))} - E) ds \leqq \left(1+\frac{\varepsilon}{2}\right)\varrho(\hat{e}).$$

We show in Appendix 3 (Theorem A.3.2) that such a g_0 exists. Given any x with $\|x\|>1$ and $\| \|x-\|x\|\hat{e}\|<1$, we define g on $[0, T\|x\|+1]$ by letting $g(0)=x$, $g(1)=\|x\|\hat{e}$, g constant on $[0,1]$ and $g(1)=\|x\|g_0(\|x\|^{-1}(s-1))$ for $s \in [1, T\|x\|+1]$ and define $s_{-1}, s_0, \ldots, s_k$ by $s_{-1}=0$, $s_0=1$, $s_i=\|x\|t_i+1$.

Notice that:

$$\tfrac{1}{2}\int_0^{s_k} \|\dot{g}(s)\|^2 ds + \int_0^{s_k} (\Sigma_{D(g(s))} - E) ds \leqq C + \left(1+\frac{\varepsilon}{2}\right)\varrho(\hat{e})\|x\|, \tag{4.5}$$

and as x runs through the requisite set:

$$0 < C_1 < s_k\|x\|^{-1} \leqq C_2 < +\infty. \tag{4.6}$$

Step 2. Replacement of potentials by ones in C_0^∞.

On account of (4.6) and Lemma 2.1, we can, by using a little of the $\frac{\varepsilon}{2}\|x\|\varrho(\hat{e})$ still available to us, replace all potentials in a Feynman-Kac formula by ones in C_0^∞, say with support in sphere of radius R_0. Moreover, we can suppose that (4.5) remains true if $\frac{\varepsilon}{2}$ is replaced by $\frac{3\varepsilon}{4}$ and Σ by the thresholds $\tilde{\Sigma}$ associated to the replaced potentials.

Step 3. Replacement of $\sum_{i<j} V_{ij}$ by $\sum_{iDj} V_{ij}$

Inside a Feynman-Kac formula we look at all paths with $\|x+b(s)-g(s)\|<R$ for $0\leqq s\leqq s_k$ where R is a parameter to be picked later. It is easy to see that the total time that it can happen that

$$\sum_{i<j} V_{ij}(s+b(s)) \neq \sum_{iD(g(s))j} V_{ij}(x+b(s))$$

is bounded independently of $\|x\|$ (just endpoints of the intervals (s_{i-1}, s_i)). Thus we get a lower bound by a formula with just $\sum_{iD(g(s))j} V_{ij}(x+b(s))$ present in the exponential.

Step 4. Translating g away

Using a Cameron-Martin formula and Jensen inequality, we replace $x+b(s)$ by $x+b(s)-g(s)$; as at the end of Sect. 3, we control the Jensen error by noting that:

$$\int_0^{s_k} \dot{g}(s)db(s) = \sum_{i=0}^{k} \dot{g}\left(\frac{s_i+s_{i-1}}{2}\right)[b(s_i)-b(s_{i-1})]$$

and that b and g are bounded.

Step 5. Lower bound on the semigroup product

The result of the above steps is a lower bound (ε' arbitrarily small):

$$\varphi(x) \geqq Ce^{-\varepsilon'\|x\|+\beta}[e^{-(s_0-s_{-1})H_0^R-\dots-(s_k-s_{k-1})H_k^R}\chi_R](0), \tag{4.7}$$

where H_i^R is H_{D_i}, with $D_i = D(g(\frac{1}{2}(s_i+s_{i-1})))$, with Dirichlet boundary condition on the sphere of radius R and $\beta = \frac{1}{2}\int_0^{s_k} \|\dot{g}(s)\|^2 ds$.

In (4.7) we still have a lower bound if we replace H_i^R by $H_i^{R-(k-i)}$. We then note that if $H_i^{R-(k-i)}$ has ground state η_i and ground state energy α_i then:

$$\begin{aligned}\exp[-tH_i^{R-(k-i)}]\chi_{R-(k-i)} &\geqq \|\eta_i\|_\infty^{-1} \exp[-tH_i^{R-(k-i)}]\eta_i \\ &= \|\eta_i\|_\infty^{-1} e^{-t\alpha_i}\eta_i \\ &\geqq \|\eta_i\|_\infty^{-1} C' e^{-t\alpha_i}\chi_{R-(k-i)-1}\end{aligned}$$

with $C' = \inf_{|y|\leqq R-(k-i)-1} \eta(y)$. Therefore, if $R>k$ we have:

$$\varphi(x) \geqq C\exp\left[-\alpha\|x\| - \frac{1}{2}\int_0^{s_k} \|\dot{g}(s)\|^2 ds - \sum_{i=0}^{k} (s_i - s_{i-1})\alpha_i\right].$$

Step 6. Completion of the proof.

Finally, by choosing R large enough, we can be sure that:

$$|\alpha_i - \tilde{\Sigma}_{D_i}| \leqq \varepsilon''$$

with ε'' arbitrarily small. With this choice we find:

$$\varphi(x) \geqq C\exp\left[-\varepsilon'\|x\| - \left(1+\frac{3\varepsilon}{4}\right)\varrho(\hat{e})\|x\|\right],$$

completing the proof. □

5. Upper Bounds by Path Integrals

In this final section, we will illustrate how path integrals can be used to obtain upper bounds by considering the ground state of Helium. With similar methods one should be able to treat the ground state of arbitrary atoms under the usual ($\varepsilon_1 \leqq \varepsilon_2 \leqq \ldots \leqq \varepsilon_N$) assumption. To handle general N-body systems, one would need more information about Agmon geodesics that we currently possess.

We assume that H has the form (3.5) with $U \leqq 0$, $W \geqq 0$, and that:

$$\lim_{|y| \to \infty} U(y) = 0 \quad \text{and} \quad \lim_{|y| \to \infty} W(y) = 0. \tag{5.1}$$

Using an argument analogous to Lemma 3.1, (5.1) can be replaced by a weaker condition, but it is somewhat simpler to assume it, so we shall. E, ε_1 and ε_2 are as defined after (3.5) except that E is not required to be the ground state, i.e. the φ in $H\varphi = E\varphi$ need not be positive. This is because we still have:

$$|\varphi(x)| \leqq \mathbf{E}\left\{|\varphi(x+b(t))| \exp\left[-\int_0^t (V(x+b(s))-E)ds\right]\right\}. \tag{5.2}$$

We begin by proving that for any $\delta > 0$ there is a constant $C_\delta > 0$ such that for any $x = (x_1, x_2) \in \mathbb{R}^6$ we have:

$$|\varphi(x_1, x_2)| \leqq C_\delta \exp\left[-(1-\delta)\sqrt{2\varepsilon_1}|x_1|\right]. \tag{5.3}$$

To do this, note that since $\varphi \in L^\infty$ [13, 49], we need only prove (5.3) for $|x_1| > R$ for some fixed, later to be determined, R. Let:

$$\alpha \equiv \sup_{|y| \geqq R} |U(y)|.$$

By (5.1), $\alpha \to 0$ as $R \to \infty$. Fix $x = (x_1, x_2)$ with $|x_1| \geqq R$, and let T be the stopping time defined by:

$$T = \min(t_0, T_{R,1}), \tag{5.4}$$

where $t_0 > 0$ is a fixed non random number and $T_{R,i}$ is given by

$$T_{R,i}(b) = \inf\{t > 0; |x_i + b_i(t)| = R\}, \qquad i = 1, 2.$$

Since T is bounded it is allowed to replace t by T in Feynman-Kac formula and so in (5.2) (see for example [49]). For times s prior to T we have $U(x_1 + b_1(s)) \geqq -\alpha$, and since $\varphi \in L^\infty$ and $W \geqq 0$, (5.2) implies:

$$|\varphi(x)| \leqq C\mathbf{E}\left\{\exp\left[T(E+\alpha) - \int_0^T U(x_2 + b_2(s))ds\right]\right\}.$$

Since the two Brownian motions b_1 and b_2 are independent and since T depends only on b_1, we can first take the expectation over b_2 considering for a while that T is constant, say t. But note that:

$$\begin{aligned}\mathbf{E}\left\{\exp\left[-\int_0^t U(x_2 + b_2(s))ds\right]\right\} &\leqq \|e^{-th_2}\|_{\infty,\infty} \\ &\leqq C_\beta e^{t(\varepsilon_2 + \beta)},\end{aligned}$$

where $h_2=-\frac{1}{2}\Delta_2+U(x_2)$ and β is an arbitrarily small number. We have used the result of [50] that:

$$\lim_{t\to\infty}\frac{1}{t}\ln\|e^{-th_2}\|_{\infty,\infty}=\lim_{t\to\infty}\frac{1}{t}\ln\|e^{-th_2}\|_{2,2}.$$

Letting $\delta=\alpha+\beta$ and $f(x)\equiv\mathbf{E}\{T\leqq s\}$, we have:

$$\begin{aligned}|\varphi(x)|&\leqq C\mathbf{E}\{\exp[T(-\varepsilon_1+\delta)]\}\\&=C\left(\int_0^{t_0}e^{-(\varepsilon_1-\delta)s}df(s)+[1-f(t_0)]e^{-(\varepsilon_1-\delta)t_0}\right)\\&=C\left(e^{-(\varepsilon_1-\delta)t_0}+(\varepsilon_1-\delta)\int_0^{t_0}e^{-(\varepsilon_1-\delta)s}f(s)ds\right)\end{aligned}$$

by an integration by parts. Next notice that, by Levy's maximal inequality ([49, Theorem 3.6.5]) we have:

$$\begin{aligned}f(s)&\leqq\mathbf{E}\{\sup_{0\leqq u\leqq s}|b(u)|\geqq|x_1|-R\}\\&\leqq 2\mathbf{E}\{|b(s)|\geqq|x_1|-R\}.\end{aligned}$$

Thus by (3.4′) of [49]:

$$f(s)\leqq C\exp[-(|x_1|-R)^2/2s].\tag{5.5}$$

Taking t_0 to infinity we find that:

$$|\varphi(x)|\leqq C'\int_0^{+\infty}\exp[-(|r_1|-R)^2/2s-(\varepsilon_1-\delta)s]ds.$$

The integrand takes its maximum values for $s=\dfrac{|x_1|-R}{\sqrt{2(\varepsilon_1-\delta)}}$, and it is easy to see that for each $\delta'>0$ there is a constant $C_{\delta',R}$ such that the integral is bounded by

$$C_{\delta',R}\exp[-\sqrt{2(\varepsilon_1-\delta-\delta')}|x_1|].$$

Since δ' and δ are arbitrarily small, (5.3) is proven.

Now we will prove that for each $\delta>0$ there is a constant C_δ for which:

$$\begin{aligned}|\varphi(x)|\leqq C_\delta[&\exp(-\sqrt{2(\varepsilon_1-\delta)}|x_1|-\sqrt{2(\varepsilon_2-\delta)}|x_2|)\\&+\exp(-\sqrt{2(\varepsilon_1-\delta)}|x_2|-\sqrt{2(\varepsilon_2-\delta)}|x_1|)].\end{aligned}\tag{5.6}$$

Since $\varepsilon_1\leqq\varepsilon_2$, we have:

$$\begin{aligned}&\min(\sqrt{2(\varepsilon_1-\delta)}|x_1|+\sqrt{2(\varepsilon_2-\delta)}|x_2|,\sqrt{2(\varepsilon_1-\delta)}|x_2|+\sqrt{2(\varepsilon_2-\delta)}|x_1|)\\&=\sqrt{2(\varepsilon_1-\delta)}\max(|x_1|,|x_2|)+\sqrt{2(\varepsilon_2-\delta)}\min(|x_1|,|x_2|),\end{aligned}\tag{5.7}$$

so (5.6) is an Agmon metric bound (see Appendix 3).

Given (5.3), (5.6) is obviously true if $|x_1|\leqq R$ *or* $|x_2|\leqq R$ for any R, so fix R (later to be adjusted) and suppose $|x_1|>R$ and $|x_2|>R$. Again we fix $t_0>0$ and we define the bounded stopping time T by:

$$T=\min(t_0,T_R),$$

where now T_R is defined by:

$$T_R(b) = \inf\{t>0; |x_1+b_1(t)|=R \text{ or } |x_2+b_2(t)|=R\}.$$

By the same argument as before we have:

$$|\varphi(x)| \leqq \mathbf{E}\{|\varphi(x_1+b_1(T), x_2+b_2(T))| e^{T(E-2\alpha)}\}.$$

Now let:

$$T_i = \min(t_0, T_{R,i}) \qquad i=1,2,$$

where $T_{R,i}$ has been defined in (5.5). Since either $T=T_1$ or $T=T_2$ we have:

$$|\varphi(x)| \leqq \sum_{i=1}^{2} \mathbf{E}\{|\varphi(x_1+b_1(T_i), x_2+b_2(T_i))| e^{T_i(E-2\alpha)}\}. \tag{5.8}$$

The $i=1$ term in (5.8) can be dominated by a constant times:

$$\mathbf{E}\{\exp[-|x_2+b_2(T_1)| \sqrt{2(\varepsilon_1-\delta)}] e^{T_1(E-2\alpha)}\} \tag{5.9}$$

on account of (5.3). Since b_1 and b_2 are independent and T_1 depends only on b_1, we have that the conditional distribution of $b_2(T_1)$ given that $T_1=s$ is exactly the distribution of $b_2(s)$. Thus defining $f(s)$ as before we have:

$$(5.9) = \int_0^{t_0} e^{(E-2\alpha)s} g(s) df(s) + [1-f(t_0)] g(t_0) e^{(E-2\alpha)t_0}$$

with:

$$g(s) = \int \exp[-|x_2+y| \sqrt{2(\varepsilon_1-\delta)}] (2\pi s)^{-3/2} e^{-|y|^2/2s} dy.$$

Integrating by parts, taking $t_0 \to \infty$ and using (5.5), we easily find that:

$$(5.9) \leqq C_R Q_R(|x_1|, |x_2|) e^{-\alpha},$$

where $C_R>0$ is a constant, Q_R is a polynomial and

$$\alpha = \inf_{y,s}[|y|^2/2s + |x_2+y| \sqrt{2(\varepsilon_1-\delta)} + (|E|-2\alpha)s + |x_1|^2/2s].$$

But:

$$|x_2+y| \sqrt{2(\varepsilon_1-\delta)} = \min_t [|x_2+y|^2/2t + (\varepsilon_1-\delta)t]$$

and thus (with $y'=x_2+y$):

$$\alpha = \inf_{y',s,t}[(|x_1|^2 + |x_2-y'|^2)/2s + |y'|^2/2t + (|E|-2\alpha)s + (\varepsilon_1-\delta)t].$$

Recognizing $a^2/s \equiv \int_0^s (a/s)^2 dt$ as the integral of the square of a constant velocity, we see that α is exactly the minimum length of a trial Agmon geodesic that goes linearly from $x=(x_1,x_2)$ to $(0,y')$ and then linearly from $(0,y')$ to $(0,0)$. This proves (5.6). □

We remark on two facets of the above proof: first, we see the choice of the minimal value of the action (1.9) of several paths coming out explicitly in the proof. Secondly, we note that one can compute or estimate quantities like:

$$\lim_{t_0\to\infty} \mathbf{E}\{e^{-aT}\}$$

easily by noting that, as a function of x_1, this is harmonic, spherically symmetric, vanishing at infinity with the value 1 as $|x_1|$ goes to R. This links up this method of obtaining upper bounds to that exploited by the Vienna group [24].

Appendix 1: Upper Bounds by the Combes-Thomas Method, some Remarks

Besides introducing the Agmon metric, Agmon [2] has developed a new approach to upper bounds, which, because it only depends on integration by parts is more "elementary" then the Combes-Thomas [15] approach which has been used in earlier papers of this series [47, 48, 17]. However, it does not seem to us to be particularly simpler than the Combes-Thomas method (nor particularly harder!). We note however (Deift [16]) that it seems easier obtaining sharper upper bounds with Agmon's method than with the Combes-Thomas method. Our goal in this appendix is to show how Agmon metric improvements on upper bounds can be accommodated within the Combes-Thomas framework.

We consider first the case $V \to \infty$, then the N-body case and finally make a remark about boundary value problems.

Fix $H_0 = -\frac{1}{2}\Delta$ and V a continuous function with $V(x) \geqq 1$ for all $x \in \mathbb{R}^n$. Let f be a C^1 function with:

$$\tfrac{1}{2}|\nabla f|^2 \leqq V. \tag{A.1.1}$$

We want to show how to prove that $e^{(1-\varepsilon)f}\varphi \in L^2$ for all $\varepsilon > 0$ and for any distributional eigenfunction φ of $H_0 + V$ with $e^{-(1-\delta)f}\varphi \in L^2$ for some $\delta > 0$.

Since the Agmon metric ϱ obeys:

$$\overline{\lim}_{|y|\to 0} |\varrho(x+y) - \varrho(x)|/|y| \leqq \sqrt{2V(x)}$$

(by the triangle inequality), it is easy, by smoothing, to find for any $\varepsilon > 0$ a C^1 function f obeying (A.1.1) with:

$$\forall x \in \mathbb{R}^n, \qquad f(x) \geqq (1-\varepsilon)\varrho(x).$$

Thus, the assertion following (A.1.1) we can replace f by ϱ, i.e., in proving the theorem below, we can without any loss of generality assume that ϱ is C^1.

Theorem A.1.1 (Lithner [34], Agmon [1]). *Let V be a continuous real function on $\mathbb{R}^n$ which satisfies:*

$$\forall x \in \mathbb{R}^n, \qquad V(x) \geqq 1 \quad \text{and} \quad \lim_{|x|\to\infty} V(x) = \infty.$$

Let:

$$\varrho(x) = \min\left\{\int_0^1 \sqrt{2V(\gamma(s))}\,|\dot\gamma(s)|\,ds\,;\ \gamma(0) = x \text{ and } \gamma(1) = x\right\}.$$

Let $\varphi \in L^2_{\mathrm{loc}}$ satisfy $H\varphi = E\varphi$ in distributional sense where $H = -\frac{1}{2}\Delta + V$. Suppose $e^{-(1-\delta)\varrho}\delta \in L^2$ for some $\delta > 0$. Then for all $\varepsilon > 0$, $e^{(1-\varepsilon)\varrho}\varphi \in L^2$.

Remark. In [48], the Combes-Thomas method was used to prove a similar result by the $\frac{1}{2}$ was not present in the analog of (A.1.1) (nor was it known how to optimize solutions). Below, in obtaining the result with $\frac{1}{2}$, we exploit a realization of Agmon [2] that the imaginary part of $H(i\alpha)$ need not be bounded.

Proof. As explained we may replace ϱ by a C^1 function f obeying (A.1.1). Define for z real:

$$H(z)=e^{izf}He^{-izf}.$$

We will prove below that $H(z)$ has a continuation to an analytic family in the sense of Kato [29] in the strip $|\mathrm{Im}\, z|<1$. Moreover, since H has compact resolvent, so will $H(z)$. In the usual way [15, 43, 17], one concludes that the spectrum of $H(z)$ is independent of z and if $H(z)\eta=E\eta$ with $\eta\in L^2$, then $e^{i(w-z)f}\eta\in L^2$ for all w in the strip.

Next note that for α real with $|\alpha|<1$, we will prove that $H(i\alpha)$ is sectorial; Kato inequality methods easily show that C_0^∞ is a core for $H(i\alpha)$ so that:

$$H(i(1-\delta))\eta=E\eta$$

(with $\eta=e^{-(1-\delta)f}\varphi$) in distributional sense implies the same result in operator sense. Thus we reduced to proving the analyticity and sectoriality.

Since $H(z+y)=U(y)H(z)U(-y)$ for y,z real and U unitary, the usual arguments [15] imply that it is sufficient to prove analyticity in a neighborhood of $\{i\alpha;\ -1<\alpha<1\}$. Write $z=y+i\alpha$ and note that, formally:

$$\begin{aligned}H(z)&=\tfrac{1}{2}(-i\nabla-z\nabla f)^2+V\\&=H+(y^2+2i\alpha y-\alpha^2)|\nabla f|^2-y(p\cdot\nabla f+\nabla f\cdot p)+i\alpha(p\cdot\nabla f+\nabla f\cdot p),\end{aligned}$$

where we use the standard notation p for the operator $-i\nabla$.

It is obvious that so long as $\varphi,\psi\in Q(-\Delta)\cap Q(V)$ then $(\varphi, H(z)\psi)$ is analytic as a quadratic function of z, so if we prove that for all $\varepsilon>0$ there is a $\delta>0$ so that for $|\alpha|<1-\varepsilon$ and $|y|<\delta$, $H(z)$ is closed and strictly sectorial on Q, then we will have the required analyticity by type (B) methods [29].

Given (A.1.1), the following estimates are obvious:

$$\begin{aligned}|\nabla f|^2&\leqq H,\\ p\cdot\nabla f+\nabla f\cdot p&\leqq 2H.\end{aligned}\tag{A.1.2}$$

Taking δ suitably it is easy to prove from this that there exists a $\delta'>0$ so that:

$$(y^2-\alpha^2)|\nabla f|^2-y(p\cdot\nabla f+\nabla f\cdot p)\leqq(1-\delta')H,$$

which, together with (A.1.2) implies the required sectoriality and closedness. □

To apply Combes-Thomas to the N-body problem, we note the following which is "essentially" a rephrasing of [17, Theorem 5.1] (and proven there by extending the Combes-Thomas method).

Theorem A.1.2. *Let H be an N-body Hamiltonian, $H\varphi=E\varphi$ with $\varphi\in L^2$ and $E<\Sigma$. Suppose that f is a homogeneous function of degree* 1 *and that there exists a nonnegative function a so that:*

(i) $\forall x,y\in X,\quad |f(x)-f(y)|\leqq\sqrt{2}\|x-y\|\int_0^1 a(\alpha x+(1-\alpha)y)d\alpha,$

with $\|\cdot\|$ the mass weighted norm (1.7) *on X.*

(ii) *For all $x \neq 0$ in X, there is a neighborhood N_x of x in X so that for all $y \in N_x$ we have:*

$$a(y)^2 \leqq \Sigma_{D(x)} - E. \tag{A.1.3}$$

Then for any $\varepsilon > 0$, $e^{(1-\varepsilon)f}\varphi \in L^\infty$.

Remarks. 1. In [17, Theorem 5.1], an assumption is made about the gradient of f but only the integral relation is used and the proof is identical.

2. There is a $\sqrt{2}$ difference between the norm (1.7) and the one used in [17] accounting for the $\sqrt{2}$ in the condition (i).

3. The hypothesis in [17] is somewhat different from (A.1.3). If $\sqrt{2}\tilde{a}$ is the gradient of a regularized f, then (A.1.3) implies that

$$\|\tilde{a}(x)\|^2 \leqq \Sigma_{D(x)} - E. \tag{A.1.4}$$

In [17], the condition required is:

$$\|\Pi_D(\tilde{a}(x))\|^2 = \Sigma_D - E, \tag{A.1.5}$$

for all D with $D \rhd D(x)$. Since Π_D is a contraction and $D \rhd D'$ implies $\Sigma_{D'} \leqq \Sigma_D$, (A.1.4) implies (A.1.5). It appears that we have lost something by doing this, but as noted by Agmon [2], (A.1.5) implies directly that $|f(x) - f(0)| \leqq \varrho(x)$ [since geodesics γ should have tangents which for almost all s obey $\Pi_{D(\gamma(s))}\dot{\gamma}(s) = \dot{\gamma}(s)$] and ϱ (when C^1) obeys (A.1.4) (see Theorem A.3.2 below).

With this result, which is proven in [17] by Combes-Thomas methods we now prove:

Theorem A.1.3. *If $H\varphi = E\varphi$ and ϱ is the corresponding Agmon metric (recall that ϱ is E-dependent) then $e^{(1-\varepsilon)\varrho}\varphi \in L^\infty$ for all $\varepsilon > 0$.*

Proof. For each x and $\varepsilon > 0$ define

$$\Sigma_x^\varepsilon = \min_{|y-x| \leqq \varepsilon|x|} \Sigma_{D(y)},$$

and let $\varrho^{(\varepsilon)}$ be the Agmon metric with $\Sigma_{D(x)}$ replaced by Σ_x^ε. $\varrho^{(\varepsilon)}$ is homogeneous of degree 1 since Σ_x^ε is homogeneous in x of degree 0 and $\varrho^{(\varepsilon)}$ obeys (i) of Theorem A.1.2 with:

$$a^{(\varepsilon)}(x) = \sqrt{\Sigma_x^\varepsilon - E},$$

since there is a triangle inequality for the metric $d^{(\varepsilon)}(x, y)$ for which $\varrho^{(\varepsilon)}(x) = d^{(\varepsilon)}(x, 0)$. (A.1.3) for $a^{(\varepsilon)}$ is trivial if we take:

$$N_x = \{y; |y - x| \leqq \varepsilon\}.$$

Thus, for all $\delta > 0$, we have $e^{(1-\delta)\varrho^{(\varepsilon)}}\varphi \in L^\infty$.

To complete the proof, we only need that $\varrho^{(\varepsilon)}(x)$ converges to $\varrho(x)$ as ε goes to 0, uniformly on compact sets. Since:

$$|\varrho^{(\varepsilon)}(x) - \varrho^{(\varepsilon)}(y)| \leqq \sqrt{2|E|}\, \|x - y\|,$$

we have uniform equicontinuity, so it suffices to prove convergence for each fixed x.

Now, $x \to \Sigma_{D(x)}$ is lower semi-continuous, so it follows that if $\varepsilon_n \to 0$ and $x_n \to x$ then:

$$\underline{\lim}_{n\to\infty} \Sigma_{x_n}^{\varepsilon_n} \geqq \Sigma_{D(x)}. \tag{A.1.4}$$

Let $\mathscr{A}^{(\varepsilon)}$ denote the action of paths for the definition of $\varrho^{(\varepsilon)}$, i.e.:

$$\mathscr{A}^{(\varepsilon)}(\gamma) = \tfrac{1}{2}\int \|\dot{\gamma}(s)\|^2 ds + \int (\Sigma_{\gamma(s)}^{\varepsilon} - E) ds.$$

For each $\varepsilon > 0$, we pick a path γ_ε defined on $[0, s_\varepsilon]$ going from x to 0 and such that:

$$\varrho^{(\varepsilon)}(x) \geqq \mathscr{A}^{(\varepsilon)}(\gamma_\varepsilon) - \varepsilon.$$

Since $\Sigma_x^\varepsilon - E \geqq \Sigma - E \geqq 0$, and since $\int_0^{s_\varepsilon} \|\dot{\gamma}_\varepsilon(s)\|^2 ds \leqq 2\mathscr{A}^{(\varepsilon)}(\gamma_\varepsilon)$, we have uniform bounds on s_ε and $\int_0^{s_\varepsilon} \|\dot{\gamma}_\varepsilon(s)\|^2 ds$. By compactness, we can find s and a path γ with $\gamma(0) = x$, $\gamma(s) = 0$ and for some sequence ε_n going to zero, $s_{\varepsilon_n} \to s$ and $\dot{\gamma}_{\varepsilon_n} \to \dot{\gamma}$ in the weak-L^2-topology. Using the weak lower semicontinuity of the L^2-norm, (A.1.4) and Fatou's lemma, one sees that:

$$\varrho(x) \leqq \mathscr{A}(\gamma) \leqq \underline{\lim}_{\varepsilon\to 0} \mathscr{A}^{(\varepsilon)}(\gamma_\varepsilon) \leqq \underline{\lim}_{\varepsilon\to 0} \varrho^{(\varepsilon)}(x).$$

But since $\varrho^{(\varepsilon)}(x) \leqq \varrho(x)$, we have the required convergence. □

Finally we would like to say a word about the applicability of the Combes-Thomas method to boundary value problems. The Combes-Thomas method exploits ideas of analytic continuation in a group parameter very similar to those originally introduced for the study of dilation analyticity. Moreover, in order to handle embedded eigenvalues, Combes and Thomas discuss both "boosts" and dilations simultaneously in their paper. For this reason, there appears to be a common misconception (see e.g. Faris [19]) that their method intrinsically uses the dilation group which, of course, would invalidate applications to boundary value problems. However, the basic group in their method is multiplication by $e^{i\alpha f}$ for some function f; since this group leaves invariant the form domains of both the Dirichlet and Neumann Laplacians, there is no problem using the Combes-Thomas method to get fall-off of eigenfunctions in boundary value problems.

Appendix 2: Pointwise Upper Bounds

The upper bounds that Lithner [34] and Agmon [1] proved in the situation where $V \to \infty$ at infinity are only L^2-bounds, i.e. of the form $e^{(1-\varepsilon)\varrho}\varphi \in L^2$ rather than pointwise bounds.

Here we want to prove pointwise bounds. Since ϱ is not usually globally Lipschitz, the method of [17, Sect. 6] is not applicable. Originally, we proved a result similar to Theorem A.2.1 below using path integral ideas but subsequently, M. and T. Hoffmann-Ostenhof emphasized to us the applicability of Harnack inequality ideas in the context of the N-body problem (see below). With that in mind we found the proof we give below:

Theorem A.2.1. *Let us assume $H\varphi = E\varphi$ with $H = -\frac{1}{2}\Delta + V(x)$ on $L^2(\mathbb{R}^n)$ and*

$$\lim_{|x|\to\infty} V(x) = \infty.$$

Suppose f is a function for which $e^f\varphi \in L^2$ and let r be a nonnegative function which satisfies:

$$\lim_{|x|\to\infty}(|x|-r(x))=\infty .$$

Define:

$$g(x)=\inf\{f(y);\ |y-x|\leqq r(x)\}.$$

Then for $|x|$ sufficiently large we have:

$$|\varphi(x)|\leqq C_n^{-1/2}r(x)^{-n/2}e^{-g(x)}\|e^f\varphi\|_2,$$

where C_n is the volume of the unit ball in n-dimensions.

Remark. For $|x|$ small the result is clear because one knows that φ is bounded [13, 49, 30].

Proof. We can find R such that:

$$(|x|\geqq R \text{ and } |y-x|\leqq r(x))\Rightarrow V(y)\geqq E.$$

Thus using Kato's inequality:

$$\Delta|\varphi|\geqq(\operatorname{sgn}\varphi)\Delta\varphi=(V-E)|\varphi|\geqq 0$$

on the ball of radius $r(x)$ about x. Thus $|\varphi|$ is subharmonic in that ball so:

$$\begin{aligned}|\varphi(x)|&\leqq C_n^{-1}r(x)^{-n}\int_{|y-x|\leqq r(x)}|\varphi(y)|dy\\ &\leqq C_n^{-1/2}r(x)^{-n/2}\left[\int_{|y-x|\leqq r(x)}|\varphi(y)|^2dy\right]^{1/2}\\ &\leqq C_n^{-1/2}r(x)^{-n/2}e^{-g(x)}\left[\int e^{2f(y)}|\varphi(y)|^2dy\right]^{1/2}. \quad \square\end{aligned}$$

In terms of the notations of Sect. 2, it is clear that for $|y-x|\leqq 1$

$$\varrho(y)\geqq\varrho_-(x)-\sup_{|u|\leqq 1}\sqrt{2V(u)}$$

since we can always take as a trial path for the $\varrho_-(x)$ problem, the path obtained by first going in a line from 0 to $x-y$ and then the path $x-y+\gamma$ with γ a trial path for the $\varrho(y)$ problem. Thus taking $r=1$ in the above and using Theorem A.1.1 we have:

Corollary. (2.8) *holds.*

In terms of the above proof, we can describe the approach to N-body pointwise bounds which we prefer; it is essentially the approach exploited by the Vienna group in their recent work [5, 24] exploiting "Harnack inequality ideas" (also called "subsolution estimates"). The above proof obviously goes through to turn L^2 to pointwise bounds so long as for some $\delta>0$ there is a C_δ with

$$|\varphi(x)|\leqq C\int_{|x-y|\leqq\delta}|\varphi(y)|dy \qquad \text{(A.2.1)}$$

(the fact that $C=C_n^{-1}\delta^{-n}$ is irrelevant). But (A.2.1) for fairly general Schrödinger operators is a result of Trudinger [20, 54]. There is a connection between all these things and Brownian motion; indeed (A.2.1) has a Brownian motion proof [6] with only hypothesis on V

$$\lim_{\alpha\to 0}\sup_x \int_{|x-y|\leqq\alpha} |x-y|^{-(n-2)}V_-(y)dy=0 \tag{A.2.2}$$

when $n\geqq 3$ and $V_-=\max(-V,0)$.

Appendix 3: Geometry of the Agmon Metric

The Agmon metric function $\varrho(x)$, for N-body systems is a basic object since it is the rate of exponential fall-off of wave functions. In studying it, it is useful to think of it as a minimum action: given any path γ in

$$X=\left\{(x_1,\ldots,x_N)\in\mathbb{R}^{\nu N};\ \sum_{i=1}^N m_i x_i=0\right\}$$

we say that γ is L^2-rectifiable if there exists an L^2 X-valued function, say $\dot\gamma$, with:

$$\gamma(s)=\gamma(0)+\int_0^s \dot\gamma(u)du\,.$$

The action of γ is then defined by:

$$\mathscr{A}(\gamma)=\tfrac{1}{2}\int_0^t \|\dot\gamma(u)\|^2du+\int_0^t(\Sigma_{\gamma(u)}-E)du\,, \tag{A.3.1}$$

where γ is supposed to be defined on $[0,t]$ and where we used the notation Σ_x for $\Sigma_{D(x)}$. Of interest is not merely

$$\varrho(x)=\inf\{\mathscr{A}(\gamma);\gamma:[0,t]\to\mathbb{R}^{\nu N},\gamma(0)=x,\gamma(t)=0,L^2\text{-rectifiable}\} \tag{A.3.2}$$

but also the form of the minimum action path. That is because higher order asymptotics should depend on more than just ϱ; indeed, in the analysis of [32], Lieb and Simon use features of the geometry of this set up to obtain detailed asymptotics in some special regions. Here, we wish to begin the study of the form of γ and the corresponding calculation of ϱ. We will find explicit formulae for ϱ in the 3-body and in the atomic case.

Theorem A.3.1. *There exists an L^2-rectifiable path γ minimizing the action subject to $\gamma(0)=x$, $\gamma(t)=0$ (t variable). For any such path:*

$$\tfrac{1}{2}\|\dot\gamma(s)\|^2=\Sigma_{\gamma(s)}-E \tag{A.3.3}$$

for almost all s in $[0,t]$. Moreover, if $D(\gamma(s))$ is constant in some interval (s_0,s_1), then $\dot\gamma$ is constant on this interval and so γ is affine on (s_0,s_1).

Proof. Since $\Sigma_x-E\geqq\Sigma-E$, we see that $\mathscr{A}(\gamma)\geqq t(\Sigma-E)$, so that trial functions for (A.3.2) need only consider t bounded by $T_0=2\varrho(x)/(\Sigma-E)$. Let us define the set $\mathscr{S}$ by:

$$\mathscr{S}=\left\{(t,\dot\gamma);t\in[0,T_0],\dot\gamma=[0,t]\to x\right.$$
$$\left.\text{such that }\int_0^t\dot\gamma(u)du=-x\text{ and }\int_0^t\|\dot\gamma(u)\|^2du\leqq 4\varrho(x)\right\}.$$

$\mathscr{I}$ is not empty since any L^2-rectifiable path from x to the origin lies in $\mathscr{I}$ if it is defined on $[0,t]$ with $t \leqq T_0$ and if $\mathscr{A}(\gamma) \leqq 2\varrho(x)$.

Topologize $\mathscr{I}$ by saying $(t_n, \dot{\gamma}_n) \to (t, \dot{\gamma})$ if and only if $t_n \to t$ and

$$\int_0^{t_n} f(s) \circ \dot{\gamma}_n(s) ds \to \int_0^t f(s) \circ \dot{\gamma}(s) ds$$

for all L^2 X-valued function f on $[0, T_0]$ where:

$$x \circ y = \sum m_i x_i \cdot y_i$$

is the scalar product in X and $x_i \cdot y_i$ the usual scalar product in $\mathbb{R}^\nu$. In this topology $\mathscr{I}$ is easily seen to be compact and $\mathscr{A}$ is easily seen to be lower semi-continuous since $x \to \Sigma_x$ is lower semi-continuous. Thus $\mathscr{A}$ takes its minimum value on $\mathscr{I}$. (A.3.3) holds as in Proposition 2.5 by noting that $ab \leqq \frac{1}{2}(a^2 + b^2)$ has equality only if $a = b$ and exploiting the invariance of

$$\mathscr{L}(\gamma) = \int_0^t \sqrt{2(\Sigma_{\gamma(s)} - E)} \|\dot{\gamma}(s)\| ds$$

under reparametrizations.

As for the final assertion fix $s_0 < s_2 < s_3 < s_1$. We need only show that $\dot{\gamma}$ is constant on $[s_2, s_3]$. By (A.3.3), we need only prove that γ is linear on that interval since then the direction of $\dot{\gamma}$ is fixed and its magnitude is fixed by (A.3.3). The straight line $\tilde{\gamma}$ from $\gamma(s_2)$ to $\gamma(s_3)$ can only have $D(\tilde{\gamma}(s)) \neq D(\tilde{\gamma}(s_2))$ for finitely many s and thus, the length of γ can be decreased if γ is replaced by $\tilde{\gamma}$ in $[s_2, s_3]$, unless γ already equals $\tilde{\gamma}$ there. □

As we will discuss below, we believe that there are at most $N-1$ times $0 = s_0 < s_1 < s_2 < \ldots < s_j < s_{j+1} = t$ $(j \leqq N-1)$ with $\dot{\gamma}$ constant on each interval $[s_{i-1}, s_i]$, with $D(\gamma(s))$ a constant D_i on such interval if finitely many points are removed, $i = 1, \ldots, j+1$, and with $D_1 \rhd D_2 \rhd \ldots \rhd D_{j+1}$. At this point we are unable even to prove that, in general, the minimizing γ has finitely many intervals with $\dot{\gamma}$ constant on each! However, we can prove the following which we need in Sect. 4:

Theorem A.3.2. *For any $\varepsilon > 0$, there is a path $\gamma : [0, t] \to x$ from x to the origin with $\mathscr{A}(\gamma) \leqq \varrho(x) + \varepsilon$ and so that $[0, t]$ is the union of a finite number of closed intervals with $\dot{\gamma}(s)$ and $D(\gamma(s))$ constant on the interior of each of these intervals.*

Proof. We begin with some preliminary remarks. Let

$$\Pi_D = \overline{\{x \in X ; D(x) = D\}} = \{x \in X ; D \rhd D(x)\}.$$

First, if $\dot{\gamma}$ is constant on (a, b) then either $\gamma([a, b]) \subset \Pi_D$ or else $\gamma([a, b]) \cap \Pi_D$ is an empty set or a single point. Thus if we show that $[0, t]$ is a union of finitely many closed intervals on each of whose interiors $\dot{\gamma}$ is constant, then by further cutting the intervals we can arrange for $D(\gamma(s))$ to be constant.

Let γ_0 be a minimizing path for $\mathscr{A}$. Suppose that for each $\delta > 0$, we find a finite number of special open intervals in $[0, t]$ with the total length of these intervals at most δ and so that their complement is a finite union of closed intervals on whose interiors $\dot{\gamma}_0$ is constant. Let γ be the path obtained by linear interpolation of $\dot{\gamma}_0$ on each of these special open intervals. Then clearly:

$$\int_0^t \|\dot{\gamma}(s)\|^2 ds \leqq \int_0^t \|\dot{\gamma}_0(s)\|^2 ds$$

so that:

$$\mathscr{A}(\gamma) \leqq \mathscr{A}(\gamma_0) + \delta\sqrt{-2E}$$

and the theorem follows.

We say that s_0 is a boundary point of type D_0 if $D(\gamma_0(s_0)) = D_0$ and if $\dot{\gamma}_0(s)$ is not constant near s_0. Suppose that $s_0 < s_1 < s_2$ are three boundary points of type D_0. Then we claim it cannot happen that $D(\gamma_0(t)) \rhd D_0$ for all $t \in [s_0, s_1]$. For if $D(\gamma_0(t)) \rhd D_0$, then $\Sigma_{\gamma_0(t)} \geqq \Sigma_{D_0}$ and thus the action can only be decreased by making γ_0 linear on $[s_0, s_1]$ which would imply that s_1 is not a boundary point of type D_0.

Now, $\|\gamma(\cdot)\|$ is continuous and non-vanishing on $[0, t-\delta/2]$, so it has a minimum value, say ε. Let $\tilde{D}$ be a decomposition with two clusters. If $D(\gamma_0(s)) = \tilde{D}$ for $0 \leqq s \leqq t - \delta/2$, then the distance between individual particles is bounded away from zero independently of s. If $D(\gamma_0(t) \not\rhd \tilde{D}$ for some $t > s$, it must happen that two particles in distinct clusters of $\tilde{D}$ come together. Since $\|\dot{\gamma}(\cdot)\|$ is bounded by (A.3.3), we see that there is a finite time necessary for this to happen. Combining this with the three time result in the last paragraph, we see that in $[0, t-\delta/2]$ there can be only finitely many boundary points of type $\tilde{D}$. Thus, in this interval, there are only finitely many boundary points of type for a D with two clusters.

About each such point remove an open interval so that the total size of these intervals is $\delta/4$. Let I be $[0, t-\delta/2]$ with these intervals removed.

Let $\tilde{D}'$ be a decomposition with three clusters. Consider all $s \in I$ with $D(\gamma(s)) = \tilde{D}'$. We claim that the minimum intercluster distance in such $\gamma(s)$ must be bounded from below since I is compact and there are no two cluster boundary points in I. Thus, as in the two cluster argument, there are finitely many boundary points of type $\tilde{D}'$ in I. Proceeding inductively, we find a finite number of open intervals of total size δ containing all boundary points. This completes the proof. □

Having established existence, we should say a word about uniqueness. Uniqueness need not hold; indeed a sign of non-uniqueness is non-smoothness of $\varrho(x)$ at points where Σ_x is smooth. For example, in the two electron atomic case (see below) on $\mathbb{R}^{2\nu}$ ($N=3$) we have:

$$\varrho(x_1, x_2) = \sqrt{\varepsilon_1}\max(|x_1|, |x_2|) + \sqrt{\varepsilon_2}\min(|x_1|, |x_2|),$$

where $\varepsilon_1 < \varepsilon_2$. If $x_1 \neq x_2$ and both are non-zero, Σ_x will be smooth but ϱ is not smooth at points with $|x_1| = |x_2|$. Thus, there should be a non-unique geodesic [from $x = (x_1, x_2)$ to the origin] at points with $|x_1| = |x_2| \neq 0$ and $x_1 \neq x_2$. Indeed, the path given in Sect. 3 and the path obtained by interchanging the roles of r_1 and r_2 are both geodesic for this problem.

There are even more extreme cases on non-uniqueness. For example consider three particles of mass 1 and suppose only the thresholds Σ_2 and Σ_3 are non-zero and these thresholds and the energy E obeys (we use the notation Σ_k for Σ_{D_k} with $D_k = \{\{i,j\},\{k\}\}$)

$$-E + \Sigma_2 < 3(-\Sigma_2) \tag{A.3.4}$$

and:
$$\alpha = \sqrt{\tfrac{4}{3}(-E+\Sigma_3)} = \sqrt{-\Sigma_2} + \sqrt{\tfrac{4}{3}(-E+\Sigma_2)} = \beta\,. \tag{A.3.5}$$

In terms of coordinates $r_{12} = x_1 - x_2$, $R_{12;3} = x_3 - \frac{1}{2}(x_1 + x_2)$, the mass weighted norm has the form:

$$\|(r_{1,2}, R_{12;3})\|^2 = \tfrac{1}{2} r_{12}^2 + \tfrac{2}{3} R_{12;3}^2\,.$$

The straight line path from $(r_{12} = 0, R_{12;3} = \mathbf{A})$ to $(0,0)$ has length $\alpha|\mathbf{A}|$. The point of (A.3.4) is that it implies that there is a minimum length path $\gamma_{\mathbf{A}}$ from $(0, \mathbf{A})$ to the origin, which has two straight line segments; one from $(0, \mathbf{A})$ to a point with $x_1 = x_2 \neq 0$ and then from there to the origin. It will have length $\beta|\mathbf{A}|$. Since $\alpha = \beta$, both these paths have the same length, but if $\theta \in [0,1]$, the path which is a straight line from $(0, \mathbf{A})$ to $(0, \theta\mathbf{A})$ and then $\gamma_{\theta\mathbf{A}}$ will have the same length! Thus there are examples with an infinity of geodesics.

In spite of these examples, it seems likely that there is a closed set $\tilde{X} \subset X$ of codimension at least 1 so that ϱ is smooth on $X \backslash \tilde{X}$ and geodesics from $x \in X \backslash \tilde{X}$ to 0 are unique.

Next we want to consider the atomic case. As a preliminary we need a general result.

Definition. *Given any two partitions D, D', let $D \cap D'$ be the partition of intersections of the clusters in D and D' (i.e. $D \cap D' \rhd D$ and $D \cap D' \rhd D'$ and it is the maximal partition with this property).*

Theorem A.3.3. *Let $\tilde{\varrho}(x)$ be a function on X with $\tilde{\varrho}(0) = 0$ and obeying:*

$$|\tilde{\varrho}(x) - \tilde{\varrho}(y)| \leqq \sqrt{2}\,\|x-y\| \sqrt{\Sigma_{D(x)\cap D(y)} - E}\,. \tag{A.3.6}$$

Then $\tilde{\varrho} \leqq \varrho$ where ϱ is the Agmon metric.

Proof. Let γ be a path from x to 0 for which there exists $0 = t_0 < t_1 < \ldots < t_k$ with $\dot{\gamma}(s)$ and $D(\gamma(s))$ constant on each interval (t_{i-1}, t_i), $i = 1, \ldots, k$. Now fix i and let $x = \gamma(t_{i-1})$, $y = \gamma(t_i)$, and $D_i = D(\gamma(\frac{1}{2}(t_{i-1} + t_i)))$. Then $D_i \rhd D(x)$ and $D_i \rhd D(y)$ so that $D_i \rhd D(x) \cap D(y)$ and $\Sigma_{D_i} \geqq \Sigma_{D(x)\cap D(y)}$. Thus:

$$\begin{aligned}\int_{t_{i-1}}^{t_i} \sqrt{2(\Sigma_{D_i} - E)}\,\|\dot{\gamma}(s)\|\,ds &\geqq \sqrt{2}\sqrt{\Sigma_{D_i} - E}\,\|x-y\| \\ &\geqq \sqrt{2}\sqrt{\Sigma_{D(x)\cap D(y)} - E}\,\|x-y\| \\ &\geqq |\varrho(\gamma(t_i)) - \varrho(\gamma(t_{i-1}))|\,.\end{aligned}$$

Consequently:

$$\tilde{\varrho}(x) \leqq \ell(\gamma)\,,$$

where $\ell(\gamma)$ is the length of γ in the Agmon metric. Minimizing over all such γ and using Theorem A.3.2, the result follows. □

Theorem A.3.4. *Consider an $N+1$ body system with particles $0, 1, \ldots, N$ with masses $m_0 = \infty$ and $m_i = \frac{1}{2}$, $i = 1, \ldots, N$. Suppose that there are numbers:*

$$0 \leqq \varepsilon_1 \leqq \varepsilon_2 \leqq \ldots \leqq \varepsilon_N$$

so that:

$$-\Sigma_D=\varepsilon_{j+1}+\ldots+\varepsilon_N,$$

where j is the total number of particles in clusters other than the one containing particle 0 (i.e. the binding energy only depends on the number of particles in the same cluster as 0 and ε_i is the removal energy of the i-th particle starting from all particles bound). Given an N-tuple $(x_1,\ldots,x_N)\in x=\mathbb{R}^{N\nu}$ define r_1 to be the maximum of the $|x_i|$, r_2 to be the next largest, etc. .... Then:

$$\varrho(x_1,\ldots,x_N)=\sum_{i=1}^{N}\sqrt{\varepsilon_i}r_i\equiv\tilde{\varrho}(x_1,\ldots,x_N).$$

Proof. Let us begin by finding a path with action $\sum_{i=1}^{N}\sqrt{\varepsilon_i}r_i$ which will show that $\varrho\leqq\tilde{\varrho}$. Without any loss of generality we can renumber the particles so that:

$$|x_1|\geqq|x_2|\geqq\ldots\geqq|x_N|.$$

Define $t_1,\ldots,t_N$ by $t_i=|x_i|/\sqrt{4\varepsilon_i}$ $i=1,\ldots,N$. By the ordering of the $|x_i|$ and the ε_i we have that

$$0\leqq t_N<\ldots\leqq t_1. \tag{A.3.7}$$

Let:

$$y_i(s)=\begin{cases}(1-s/t_i)x_i & 0\leqq s\leqq t_i\\ 0 & t_i\leqq s\leqq t_1\end{cases}.$$

Notice that on $[0,t_i]$ we have $|\dot{y}_i(s)|=\sqrt{4\varepsilon_i}$. Now let:

$$\gamma(s)=(y_1(s),\ldots,y_N(s)),\qquad s\in[0,t_1].$$

Then:

$$D(\gamma(s))=\{\{0,N,N-1,\ldots,i\},\{i-1\},\ldots,\{1\}\}$$

whenever $s\in(t_i,t_{i-1})$, and so, in that interval:

$$\Sigma_{\gamma(s)}-E=\varepsilon_1+\ldots+\varepsilon_{i-1}=\sum_{j=1}^{i-1}\frac{m_j}{2}\|\dot{y}_j\|^2.$$

Thus:

$$\begin{aligned}\mathscr{A}(\gamma)&=2\int_0^{t_1}\sum_j\frac{m_j}{2}\|\dot{y}_j\|^2ds\\&=\sum_j\tfrac{1}{2}(\sqrt{4\varepsilon_j})^2t_j\\&=\varrho(x),\end{aligned}$$

and so $\varrho\leqq\tilde{\varrho}$. To complete the proof, let us show that $\tilde{\varrho}$ obeys (A.3.6). Let:

$$C_0(x)=\{i\in\{1,\ldots,N\};x_i=0\},$$

[i.e. $C_0(x)$ is the set of particles in the cluster of $D(x)$ containing 0] and let $n(x)$ be the number of elements of $C_0(x)$. Then clearly, for all but finitely many α in [0, 1] we have:

$$C_0(\alpha x+(1-\alpha)y)=C_0(x)\cap C_0(y)$$

[exceptional values are given by α for which $\alpha x+(1-\alpha)y=0$ although $x\neq 0$ and $y\neq 0$]. Since $\Sigma_x=\sum_{j=N-n(x)}^{N-1}\varepsilon_{j+1}$, we conclude that:

$$\Sigma_{\alpha x+(1-\alpha)y}=\Sigma_{D(x)\cap D(y)}$$

except for a finite set of α. Moreover, it is easy to see that $\tilde{\varrho}(\alpha x+(1-\alpha)y)$ is smooth in α for all but a finite number of values of α [exceptional values are those where $|\alpha x_i+(1-\alpha)y_i|=|\alpha x_j+(1-\alpha)y_j|$ for some $i\neq j$ with the equality not holding for all α] and:

$$\frac{d}{d\alpha}\tilde{\varrho}(\alpha x+(1-\alpha)y)\leqq\sqrt{2}\|x-y\|\Sigma_{\alpha x+(1-\alpha)y}\,.$$

Thus, integrating $\frac{d\tilde{\varrho}}{d\alpha}$, (A.3.6) holds. □

In studying geodesics, there are several useful pictures of how geodesics look at points where $\dot{\gamma}$ and D change. We want to describe two pictures: the optical analogy and the mechanical analogy. The basis of the optical analogy is:

Proposition A.3.5. *Consider* $\mathbb{R}^2$ *with the usual Euclidean structure and coordinates. Suppose* $\varepsilon_1,\varepsilon_2>0$ *and that lengths of paths are determined by multiplying the Euclidean length by* $\sqrt{\varepsilon_1}$ *if the path is contained in the axis* $\{(x,y)\in\mathbb{R}^2; y=0\}$ *and otherwise by* $\sqrt{\varepsilon_1+\varepsilon_2}$. *Let* θ *be defined by* $\tan\theta=\sqrt{\varepsilon_2/\varepsilon_1}$, *and suppose* $x,y>0$. *Then the geodesic form* (x,y) *to* $(0,0)$ *is a straight line if and only if* $y/x\geqq\tan\theta$. *If* $\frac{y}{x}<\tan\theta$, *then the geodesic consists of two straight line segments with intermediate point* $(x_0,0)$ *determined by the condition that the angle between these segments is* θ *(see Fig. 1). Moreover, in that case the length of the geodesic is:*

$$\ell=\sqrt{\varepsilon_1}x+\sqrt{\varepsilon_2}y \tag{A.3.8}$$

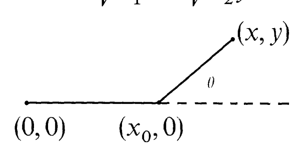

Fig. 1

The proof is a simple exercise of elementary calculus because clearly, we have only to minimize the length of all paths shown in Fig. 1, i.e.,

$$\beta(x_0)=\sqrt{\varepsilon_1}x_0+\sqrt{\varepsilon_1+\varepsilon_2}\sqrt{(x-x_0)^2+y^2}$$

subject to $x_0\geqq 0$. So it is left to the reader.

Equation (A.3.8) helps explain why in Theorem A.3.4, it is $\sqrt{\varepsilon_1}$ that enters even though the basic lengths are multiplied by square roots of sums of ε_i's. We call this result the optical analogy because it says that the angle of incidence θ is exactly that at which Snell's law predicts that the refracted wave will move along the surface. If we think of the plane in an N-body system as limit of thin slabs, this is exactly the condition for light to stay in the slab.

The above result determines the angle between successive segments of an Agmon geodesic.

The mechanical analogy is based on the fact that X consists of sets of points $(x_1, \ldots, x_N)$ with $\sum_{i=1}^{N} m_i x_i = 0$. Thus, a path γ in X consists of N paths γ_i in $\mathbb{R}^\nu$ and at points s where $\dot{\gamma}(s)$ exists we have:

$$\sum_{i=1}^{N} m_i \dot{\gamma}_i(s) = 0\,. \tag{A.3.9}$$

This can be thought of as momentum conservation and (A.3.3), which holds for minimum *action* paths, as energy conservation. An increase in the number of clusters in $D(\gamma(s))$ represents some clusters "decaying" and there is an energy *gain* in this. Suppose at some s_0 we have the breakup of a single cluster $\tilde{C}$ into two clusters C_1 and C_2. Using the fact that one is minimizing an action, it is easy to see that the velocities of all other clusters must be fixed as s passes through s_0, or else one could decrease the putative minimum action. This consistency of the other velocities can be seen to be precisely equivalent to the angle condition in the optical analogy!

Next we want to compute exactly the Agmon geodesic in the three body case. The following is critical to our analysis:

Proposition A.3.6. *Let D_0 be a partition with precisely two clusters C_1 and C_2, and let $\Pi_D = \{x \in X\,; D(x) = D_0\}$. If there is an $x \in \Pi_D$, $x \neq 0$ so that the straight line from x to 0 is not an Agmon geodesic, then that is true for all $x \in \Pi_D$ and moreover, any minimum length path $\gamma(s)$ from x to 0 does not lie in Π_D for small s.*

Proof. The underlying Riemannian structure is invariant under scaling and under simultaneous rotation of *all* the x_i. This shows that given any $y \in \Pi_D$ with $\|y\| = 1$ and any path of length $\ell(\gamma)$ from y to the origin, there is a path $\tilde{\gamma}$ from a given $x \in \Pi_D$ to the origin with length $\ell(\tilde{\gamma}) = \|x\| \ell(\gamma)$, obtained from γ by scaling and rotation. Moreover γ lies in Π_D if and only if $\tilde{\gamma}$ lies in Π_D. This proves the first result.

Now, for $x \in \Pi_D$, let $\alpha\|x\|$ be the length of the straight line from x to 0, and let $\beta\|x\|$ be the Agmon distance from x to 0. By hypothesis $\beta < \alpha$. If a geodesic from x to the origin begins in Π_D, then letting $g(s) = \gamma(s)$ for small s, we see that:

$$\beta\|x\| = \alpha\|x - y\| + \beta\|y\|\,,$$

which is inconsistent with $\beta < \alpha$ and the triangle inequality. Thus all geodesics do not begin in Π_D. □

Corollary A.3.7. *Let γ be an Agmon geodesic from a point $x \in X$ in the three body case to the origin. The γ can be choosen to either be a straight line or a broken line of two segments, one from x to some $y \in \Pi_D$ for some $D = \{\{i,j\}, \{k\}\}$ and the other in Π_D.*

Proof. Consider each partition $D_k=\{\{i,j\},\{k\}\}$ in two clusters and the corresponding $\Pi_k=\Pi_{D_k}$. If the geodesic from points in Π_k to 0 cannot be choosen as straight lines in Π_k we call D_k ineffective, otherwise we call D_k effective. Let γ be a geodesic from $x\in X$ to the origin 0. If this geodesic crosses an ineffective plane, then, by the above Proposition, the path cannot shift to lying in this plane so it must pass directly through and remain straight (otherwise, we can shorten length in an obvious way). Let x_0 be the first point on the geodesic lying on an effective plane. The path must be linear from x to x_0, and then can be choosen (perhaps by changing γ: see the second example of non-uniqueness!) to be linear from x_0 to 0. □

Now we can describe the metric and geodesic in the three-body case. Let m_1, m_2, m_3 be the masses and let:

$$\mu_1=(m_2^{-1}+m_3^{-1})^{-1} \quad \text{and} \quad M_1=[m_1^{-1}+(m_2+m_3)^{-1}]^{-1},$$

and similarly for μ_2, M_2, μ_3 and M_3. Let Σ_1 be the threshold for the partition $D_1=\{\{1\},\{2,3\}\}$ and similarly for Σ_2 and Σ_3. Given $x=(x_1,x_2,x_3)\in X$, let:

$$y_1=|x_2-x_3| \quad \text{and} \quad z_1=|x_1-(m_2+m_3)^{-1}(m_2x_2+m_3x_3)|$$

and similarly for y_2, z_2, y_3 and z_3. Note that:

$$\mu_i y_i^2+M_i z_i^2\equiv d(x)^2$$

is independent of i and is the square of the mass weighted norm of x.

Define:

$$\varrho_1(x)=\begin{cases}\sqrt{-2E}\,d(x) & \text{if } (-\Sigma_1)\mu_1 y_1^2 \geqq (\Sigma_1-E)M_1 z_1^2\\ \sqrt{M_1}\,z_1\sqrt{2(\Sigma_1-E)}+\sqrt{\mu_1}\,y_1\sqrt{2(-\Sigma_1)} & \text{otherwise}\end{cases}$$

and $\varrho_2(x)$ and $\varrho_3(x)$ similarly. Then:

Theorem A.3.8. *In the three-body case we have:*

$$\varrho(x)=\min(\varrho_1(x),\varrho_2(x),\varrho_3(x)).$$

Remark. This means that the upper bound found in [17, Sect. 8] is optimal, at least for the ground state.

Proof. We consider all paths from x to the origin in two linear segments with $x'\in\Pi_{D_i}$ as intermediate point. By the above Corollary we know that we can look for geodesics in this class. Now, by Proposition A.3.5 a geodesic will have intermediate point x' different from 0 if and only if $(-\Sigma_i)\mu_i y_i^2 \leqq M_i z_i^2(\Sigma_i-E)$, in which case its length is $\sqrt{M_i}z_i\sqrt{2(\Sigma_i-E)}+\sqrt{\mu_i}\,y_i\sqrt{2(-\Sigma_i)}$. Otherwise $x'=0$ and the result is clear. □

Given the above complicated form for the three body case, one expects that the general N-body case will be ghastly. The natural conjecture is that the number of functions needed in the general case is the number of strings, i.e. sets of partitions $D_1, D_2, \ldots, D_n$ with $1,2,\ldots,N$ clusters respectively and with $D_1 \rhd D_2 \rhd \ldots \rhd D_N$ (e.g. there are 18 strings when $N=4$). It seems to us possible that the following is true: "the Agmon geodesic γ can always be choosen so that there is a string $D_1 \rhd \ldots \rhd D_N$

and times $\theta = t_0 \leqq t_1 \ldots \leqq t_{N-1}$ so that $\dot{\gamma}$ is constant on each interval (t_{i-1}, t_i) and for all but finitely many s in that interval $D(\gamma(s)) = D_{N+1-i}$". The proof of this would go a long way towards finding an explicit formula for ϱ in the N-body case.

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Note added in proof. S. Agmon has emphasized to us that although stated in his announcement in terms of global hypotheses on V, his passage to pointwise bounds only requires local hypotheses on V.