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Pointwise Bounds on Eigenfunctions and Wave Packets in N-Body Quantum Systems. VI. Asymptotics in the Two-Cluster Region

ELLIOTT H. LIEB AND BARRY SIMON*

Departments of Mathematics and Physics, Princeton, New Jersey 08544

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We study the asymptotic behavior of the ground-state wave function of multiparticle quantum systems without statistics in that region of configuration space where the particles break up into two well-defined clusters very far apart. One example of our results is the following: consider a system of N particles moving in three dimensions with rotationally invariant two-body potentials which are bounded and have compact support. Let $D = \{C_1, C_2\}$ be a partition into two clusters so that $H(C_1)$ and $H(C_2)$ have discrete ground states η_1 and η_2 of energy ϵ_1 and ϵ_2. Suppose that $\Sigma = \epsilon_1 + \epsilon_2 = \inf \sigma_{\mathrm{ess}}(H)$ and that H has a discrete ground state φ of energy E. Let ζ_1 and ζ_2 denote internal coordinates for the clusters C_1 and C_2 and let R be the difference of the centers of mass of the clusters. Let $\mu = M_1 M_2/M_1 + M_2$ with M_i the mass of clusters C_i and define k by $k^2/2\mu = \Sigma - E$. Then as $R \to \infty$ with $|\zeta_i|$ bounded, we prove that

$$\varphi(\zeta_1, \zeta_2, R) = c\eta(\zeta_1)\eta(\zeta_2)e^{-kR}R^{-1}(1 + O(e^{-\gamma R}))$$

for some $\gamma, c > 0$. We prove weaker conclusions under weaker hypotheses, including results in the atomic case.

1. INTRODUCTION

During the past ten years, there has been extensive study of the asymptotics of discrete eigenfunctions of multiparticle Schrödinger operators. Recently, with work of Hoffman-Ostenhof [5], Deift *et al.* [4], Agmon [1], and Carmona and Simon [3], there has been a definitive solution of the problem of finding the leading asymptotics; specifically, if $\varphi(x_1, \ldots, x_N) = \varphi(x_i)$ is the ground state (without statistics) of an N-particle system

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viewed as a function on the plane with $\Sigma_1^N m_i x_i = 0$, then

$$\lim_{\substack{|x|\to\infty \\ x/|x|\to c}} -|x|^{-1}\ln[\varphi(x_i)] = \rho(c)$$

with ρ an explicit function of c and the various masses and thresholds ("the Agmon metric"). Here $|x| = [\Sigma m_i x_i^2]^{1/2}$ on the plane with $\Sigma m_i x_i = 0$. Even though ρ is a complicated function (described in Section 2) it only depends on the limiting value of $x/|x|$. One cannot hope that asymptotics past the leading order will only depend on this limiting value. For example, let $\varphi(x_1, x_2)$ be the ground state of a two-electron system with infinite nuclear mass. Fix two distinct values of x_2 and consider

$$\lim_{\substack{|x_1|\to\infty \\ x_1/|x_1|=\hat{c}}} \varphi(x_1,a)/\varphi(x_1,b). \tag{1.1}$$

Despite the fact that $|(x_1,a)|^{-1}(x_1,a)\to(\hat{c},0)$ and the same limit for b, one does not expect that the ratio in (1.1) goes to 1; rather it is reasonable to expect that its limit is $\eta(a)/\eta(b)$ with η the ground state for a one-electron system. It is exactly results of this genre that we prove in this paper. Our interest was stimulated by related conjectures (described below) of J. Morgan and T. Hoffman-Ostenhof.

More generally, consider an N-body system (without statistics) and suppose that the Hamiltonian, H, has a discrete (automatically nondegenerate and positive) ground state, φ. Let $D = \{C_1, C_2\}$ be a breakup of $\{1,\ldots,N\}$ into two pieces and use coordinates R, ζ_1, ζ_2 where R is the difference of the positions of the centers of mass of the two clusters and ζ_i is a set of "internal" coordinates for cluster C_i, i.e., a set of coordinate differences of particles in C_i which is large enough for $\zeta = (\zeta_1, \zeta_2)$ and R to be a complete coordinate system for the N-body system with center of mass removed. Let $H(C_i)$ be the Hamiltonian of cluster C_i with its center of mass motion removed and suppose that each $H(C_i)$ has a discrete ground state, η_i. Write $\eta(\zeta) = \eta_1(\zeta_1)\eta_2(\zeta_2)$.

The natural extension of (1.1) is that for fixed ζ, ζ':

$$|\varphi(\zeta,R)/\varphi(\zeta',R) - \eta(\zeta)/\eta(\zeta')| \to 0 \tag{1.2}$$

as $R\to\infty$.

Under an extra condition on masses and thresholds which we describe in Section 2, we will prove (1.2) in Sections 3 and 4. In Section 3, we treat the case where the two-body potentials have compact support and obtain (1.2) with an error which is $O(e^{-aR})$ for $a > 0$. In Section 4, we prove that if the two-body potentials are $O(r^{-\alpha})$ at infinity with $\alpha \geq 1$, then (1.2) holds with errors which are $O(R^{-(\alpha-1)})$. In Section 5, we return to the case of potentials of compact support and prove the stronger:

$$\varphi(\zeta, R)/\left[|R|^{-(\nu-1)/2}e^{-kR}\right] \to C\eta(\zeta) \tag{1.3}$$

for ζ fixed and $R \to \infty$ where $C \neq 0$, ν is the underlying dimension of the configuration space for one particle and $k = \sqrt{2\mu(\delta E)}$ with μ the reduced mass of the two clusters and δE the difference of the energy, E, of φ (i.e., $H\varphi = E\varphi$) and the energy, Σ_D, of η (i.e., $[H(C_1) + H(C_2)]\eta = \Sigma_D\eta$).

We remark here, that the extra condition that we need on the masses and thresholds automatically holds if Σ_D is the lowest threshold of the system, i.e., $\Sigma_D = \inf \sigma_{\mathrm{ess}}(H)$. Moreover, as we explain in Section 2, (1.2) should be false in many cases where the extra condition fails. Some geometry associated to the extra condition is further described in the Appendix.

For the case of an atom with C_2 a single electron (our extra condition holds here because of the remark at the start of the last paragraph), J. Morgan and T. Hoffman-Ostenhof made the related conjecture

$$\varphi(\zeta, R)\Big/\left[\int |\varphi(\zeta, R)|^2 d\zeta\right]^{1/2} \to \eta(\zeta) \tag{1.4}$$

as $R \to \infty$ in $L^2(d\zeta)$ norm. While we have not succeeded in proving this in the atomic case (where we only handle things for fixed *finite* ζ), we do prove (1.4) in the case of potentials of compact support; see Section 5.

It is a pleasure to thank John Morgan III and T. Hoffman-Ostenhof for telling us of their conjecture and thereby stimulating our interest in these questions.

2. The Agmon Metric

In this section, we describe in detail the extra condition we need to prove (1.1) and explain why some kind of extra condition is needed. To do this, we need to recall the definition of the metric introduced by Agmon [1] and its interpretation in terms of path integrals by Carmona and Simon [3].

For each breakup, $D = \{C_1, \ldots, C_k\}$ of $\{1, \ldots, N\}$ into k clusters, there is a coordinate system (ζ_D, R_D) similar to that used in Section 1 for $k = 2$. $R_D \in R^{\nu(k-1)}$ is some set of differences of centers of mass of the clusters and $\zeta_D \subset R^{\nu(N-k)}$ is some set of differences of coordinates in the same cluster. We can think of $\{R_D\}$ as $\{(R_1, \ldots, R_k) | \Sigma M(C_i)R_i = 0\}$ with $M(C_i)$ the mass of cluster C_i and R_i the center of mass of cluster R_i. On this set, we introduce the distance:

$$d_D(R_D, R_D') = \left(2\Sigma M(C_i)(R_i - R_i')^2\right)^{1/2}.$$

Now let $\pi_D = \{x = (\zeta_D, R_D) | \zeta_D = 0\}$ and

$$\tilde{\pi}_D = \pi_D \setminus \bigcup \{\pi'_D | D' \text{ refines } D\}$$

$\tilde{\pi}_D$ is precisely the set of $x = (x_1, \ldots, x_N)$ where D is the exact clustering resulting by lumping together those i,j with $x_i = x_j$. Finally, let Σ_D be the minimum energy obtained by replacing all pair potentials, V_{ij} with i,j in different clusters by zero.

The Agmon metric $\rho(x)$ is defined as follows: Fix $E < \Sigma = \min_D \Sigma_D$. Consider all piecewise linear paths from x to 0. One can break up any such path into segments S_i whose interior lies in some $\tilde{\pi}_{D_i}$. We define the length of such segment as $(\Sigma_D - E)^{1/2} d_D(R, R')$ if $(R, \zeta = 0), (R', \zeta = 0)$ are the initial and final points of S_i in the (R_{D_i}, ζ_{D_i}) coordinate system. The length of the path is the sum of the lengths of segments and $\rho(x)$ is the minimum of the length of all paths from x to 0.

The Agmon metric is of interest because of the following:

THEOREM 2.1 (upper bound [1], lower bound [3]). *For the ground-state wave function, φ, and any $\epsilon > 0$, there exist constants C, D so that*

$$Ce^{-(1+\epsilon)\rho(x)} \leq \varphi(x) \leq De^{-(1-\epsilon)\rho(x)}, \tag{2.1}$$

where ρ is the Agmon metric with E the energy of the ground state.

Remark. An upper bound on $|\varphi(x)|$ holds for any L^2 eigenfunction [1].

The condition we will need to prove (1.1) is:

DEFINITION. A breakup D into two clusters is called *regular* if and only if for any fixed $R \in R^{\nu}$, the minimum of $\rho(x)$ on the plane $\{(R_D, \zeta_D) | R_D = R\}$ occurs at the point $\zeta_D = 0$.

Remark. By scaling and rotational invariance, the condition for one $R \neq 0$ implies it for all $R \neq 0$.

If D determines the bottom of the continuum, then we have that:

PROPOSITION 2.2. *If $\Sigma_D = \Sigma = \min_{D'} \Sigma_{D'}$, then D is regular.*

Proof. Let $\tilde{\rho}$ be defined analogously to the Agmon metric, but with $\sqrt{2}\,(\Sigma_D - E)^{1/2} d_D(R, R')$ replaced by $\sqrt{2}\,(\Sigma - E)^{1/2} d_D(R, R')$. Clearly, since $\Sigma = \min_D \Sigma_D$

$$\tilde{\rho}(x) \leq \rho(x) \tag{2.2}$$

for any x. Moreover, since $\tilde{\rho}$ is geodesic distance in a constant Riemannian metric, the geodesics are straight lines and

$$\frac{1}{2}\tilde{\rho}(x)^2 = \left(\sum_{i=1}^{N} m_i x_i^2\right)(\Sigma - E) \equiv \langle x, x \rangle.$$

Since the directions $(R_D, 0)$ are orthogonal to the $(0, \zeta_D)$ directions in the $\langle\ ,\ \rangle$ inner product, the minimum of $\tilde{\rho}$ on the plane $\{(R_D, \zeta_D) | R_D = R\}$ occurs at $\zeta_D = 0$. If we prove that $\tilde{\rho}(R_D, 0) = \rho(R_D, 0)$, we have proven regularity of D.

But, since $\Sigma = \Sigma_D$, the straight line from $(R_D, 0)$ to $(0,0)$ has ρ-length which equals $\tilde{\rho}(R_D, 0)$. So, by (2.2), $\rho(R_D, 0) = \tilde{\rho}(R_D, 0)$. $\square$

In our study of (1.1), regularity will enter through the following:

THEOREM 2.3. *Suppose that $D = \{C_1, C_2\}$ is a regular clustering and that H has a normalized ground state, φ, and $H(C_1) + H(C_2)$ has a normalized ground state η. Let $\varphi_R(\zeta) \equiv \varphi(R, \zeta)$ in the coordinate system (R_D, ζ_D) associated to D. Then, for any δ, there exists a C_δ with*

$$\langle \eta, \varphi_R \rangle \geq C_\delta e^{-2\delta|R|} [\langle \varphi_R, \varphi_R \rangle]^{1/2} \tag{2.3}$$

with $\langle f, g \rangle \equiv \int \overline{f(\zeta)} g(\zeta)\, d\zeta$.

Proof. We use the bounds in Theorem 2.1. For $|\zeta| \leq 1$, $\rho(R, \zeta) \leq \rho(R, 0) + C$ (for take a trial path of a straight line from (R, ζ) to $(R, 0)$ and then a geodesic from $(R, 0)$ to $(0,0)$). Since $\eta(\zeta)$ has a strictly positive lower bound on $\{\zeta \,|\, |\zeta| < 1\}$ [8], we obtain

$$\langle \eta, \varphi_R \rangle \geq C_{1,\delta} e^{-\rho(R,0) - \delta|R|}$$

from the lower bound in (2.1) and the contribution of $|\zeta| < 1$ to the integrals.

Next we claim that, *by regularity*

$$\rho(\zeta, R) \geq \rho(R, 0) + a(|\zeta| - b|R|)_+ \tag{2.4}$$

for suitable $a, b > 0$, with $(x)_+ \equiv \max(x, 0)$. Accepting (2.4) for the moment, the upper bound in (2.1) implies that

$$\langle \varphi_R, \varphi_R \rangle \leq D^2 e^{-2(1-\epsilon)\rho(R,0)} \int e^{-a(|\zeta| - b|R|)_+}\, d\zeta. \tag{2.5}$$

But the integral in (2.5) is for suitable m

$$\text{const}\left[\int_0^{b|R|} |\zeta|^m d|\zeta| + \int_{b|R|}^{\infty} |\zeta|^m e^{-a(|\zeta| - b|R|)} d|\zeta| \right],$$

which is bounded by $C(1 + (b|R|)^{m+1})$ and thus choosing ϵ suitably

$$\langle \varphi_R, \varphi_R \rangle \leq C_{2,\delta} e^{-2\rho(R,0) + 2\delta|R|}$$

(2.3) thus follows.

This leaves the proof of (2.4) which is where regularity enters. By (2.2), we see that

$$\rho(\zeta, R) \geq 2a|\zeta| \tag{2.6}$$

for some $a > 0$. By regularity

$$\rho(\zeta, R) \geq \rho(R, 0). \tag{2.7}$$

If we take $b = a^{-1}\rho(R,0)|R|^{-1}$ (which is independent of R), (2.4) follows. □

To explain why (1.2) will not always hold, it is useful to describe something about the Carmona–Simon [3] proof of the lower bound (2.1). For each of the trial paths in the definition of the Agmon metric, one can choose a suitable time parametrization, $\gamma(t)$ $(0 \leq t \leq T)$ and look at the contribution to a Feynman–Kac formula [8],

$$\varphi(R,\zeta) = E\left(\exp\left(\int_0^T (E - V)((R,\zeta) + Ab(s))\,ds\right)\varphi((R,\zeta) + Ab(T))\right) \tag{2.8}$$

(with b Brownian motion, $E(\cdot)$ Brownian expectation, and A a suitable matrix depending on the masses) of those paths b with $|Ab(s) - \gamma(s)| \leq D$ for some fixed D. If $L(\gamma)$ is the length of γ, by choosing D very large (depending on δ), they find

$$\varphi(R,\zeta) \geq C_\delta \exp(-(1 + \delta)L(\gamma)).$$

By minimizing over γ, the lower bound in (2.1) results. Thus one pictures the falloff of $\varphi(R,\zeta)$ coming from a particular set of paths in the expectation (2.8).

Now suppose that we consider varying (R,ζ) with $|\zeta|$ bounded and $|R| \to \infty$. If the geodesic from (R,ζ) to $(0,0)$ stays in the region with $|\zeta|$ bounded, then the potentials in the clusters will act in a Feynman–Kac formula in the dominant region of path space, so that, in effect a semigroup $e^{-T[H(C_1)+H(C_2)]}$ can be identified. For T large, the semigroup will project onto the ground state η and (1.2) should result. But, if the geodesic leaves that region, then η has nothing to do with the dominant region of phase space and so (1.2) is not reasonable.

Here is an explicit example: consider three one-dimensional particles; one, call it 0, with infinite mass; and two with masses $\frac{1}{2}$, so that

$$H = -\frac{d^2}{dx_1^2} - \frac{d^2}{dx_2^2} + V_1(x_1) + V_2(x_2) + V_{12}(x_1 - x_2).$$

We will pick V_{12} in a moment. Pick V_1 and V_2 to be attractive potentials so that the energies

$$\epsilon_i = \min \operatorname{spec}\left(-\frac{d^L}{dx_i^2} + V_i(x_i) \right)$$

obey $\epsilon_1 < \epsilon_2 < 0$ with ϵ_1/ϵ_2 very large. It is easy to compute the Agmon metric ρ' for

$$H' = H - V_{12}(x_1 - x_2)$$

since we have (2.1) and we know the asymptotic behavior of φ (it is a product function) as $|x_1|, |x_2| \to \infty$; namely,

$$\varphi \sim \exp\left(\left[\sqrt{-\epsilon_1}\, |x_1| + \sqrt{-\epsilon_2}\, |x_2| \right] \right)$$

so that

$$\rho'(x_1, x_2) = \sqrt{-\epsilon_1}\, |x_1| + \sqrt{-\epsilon_2}\, |x_2|.$$

In particular,

$$\rho'(x_1 = x_2 = a) < \sqrt{-\epsilon_1 + \epsilon_2)}\, \sqrt{2a^2}\,. \tag{2.9}$$

The inequality in (2.9) is strict, since (2.9) can be derived from the Schwarz inequality and since $\epsilon_1/\epsilon_2 \neq 1$, there is no equality. The point of (2.9) is that the right side is the length of the straight line from (a, a) to $(0, 0)$ in the assignment of lengths giving the Agmon metrics.

Now suppose that

$$V_{12}(y) = -\lambda(1 + |y|)^{-1}$$

with λ very small. Let ϵ_{12} be the (12) threshold, i.e., the minimum energy of $(-2(d^2/dx_{12}^2) + V_{12}(x_{12}))$ (the 2 comes from reduced mass considerations) and let E be the ground-state energy of H. Both ϵ_{12} and $E - (\epsilon_1 + \epsilon_2)$ will be small if λ is small. For such small λ

$$\rho(x_1 = x_2 = a) < \sqrt{-(E - \epsilon_{12})}\, \sqrt{2a^2}\,. \tag{2.10}$$

Indeed, (2.10) can be verified by explicit calculation (one finds $\rho(x_1 = x_2 = a) = |a|\left(\sqrt{-\epsilon_1} + \sqrt{-(E - \epsilon_1)}\right)$) but it also follows from (2.9) and a small argument showing uniform continuity of $\rho(x)/|x|$ in λ.

Now let $C_1 = \{0\}, C_2 = \{1, 2\}$ so that $R = \frac{1}{2}(x_1 + x_2), \zeta = (x_1 - x_2)$. (1.2) is based on the intuition that for R large, ζ bounded

$$\varphi \sim c\eta(\zeta)\exp\left(-\sqrt{2R^2}\, \sqrt{-(E - \epsilon_{12})} \right). \tag{2.11}$$

By (2.10) and (2.1), φ is much larger at infinity than the right side of (2.11).

One can check that the regularity condition we require fails in this case: The explicit formula,

$$\rho'(R,\zeta) = \sqrt{-\epsilon_1}\,|R + \tfrac{1}{2}\zeta| + \sqrt{-\epsilon_2}\,|R - \tfrac{1}{2}\zeta|$$

shows that $(d\rho'/d\zeta)|_{\zeta=0} = \frac{1}{2}(\sqrt{-\epsilon_1} - \sqrt{-\epsilon_2}) \neq 0$ so that the minimum of ρ' does not occur at $\zeta = 0$ (rather it occurs at $\zeta = 2R$). Thus, for λ small, the minimum still occurs at $\zeta \neq 0$.

Above we discussed two distinct geometric conditions:

(1) That $D = \{C_1, C_2\}$ is regular, i.e., $\rho(R,\zeta)$ with R fixed is minimized at $\zeta = 0$.

(2) That the geodesic from $(R, \zeta = 0)$ to $(0,0)$ is of the form $(R(s), \gamma(s) = 0)$.

In the Appendix, we show that (1) implies (2) so it is not surprising we only need (1) to prove (1.2) since the intuition suggests that only (2) is needed. We also give an example in the Appendix where (2) holds but (1) does not, so there are examples where one expects (1.2) to hold but where we are unable to prove it.

We close this section with a remark about the proof which explains why it is Theorem 2.3 that enters rather than some condition about the geodesic from $(R, \zeta = 0)$ to $(0,0)$. In the Feynman–Kac formula (2.8), T is a free parameter. For small T, the significant paths $(R,\zeta) + Ab(s)$ do not make it all the way from (R,ζ) to $(0,0)$ but as T reaches a critical value, T_0, the paths do reach "near" $(0,0)$ and for larger T they spend most of the time after T_0 "near" $(0,0)$. The proof of Carmona and Simon [3] and any proof exploiting conditions on geodesics to $(0,0)$ would require estimating (2.8) for $T \gtrsim T_0$ and this requires rather fine estimates on what happens when all particles are near each other (in [3], the fact that large but R-independent multiplicative errors will not invalidate (2.1) is exploited to avoid the region when particles are too close). We have not succeeded in controlling such subtle things but rather finesse this problem by choosing T small compared to T_0 but still large compared to 1. This will require an estimate on φ_R for R large and that is where Theorem 2.3 enters.

3. Asymptotics of the Ratio: Potentials of Compact Support

In this section, we want to verify (1.2) with exponentially small errors when all potentials have compact support. To avoid notational complications, we describe a special situation with three particles and then describe the general case. We will take one infinite mass particle and two particles of mass 1 so

$$H = -\tfrac{1}{2}\Delta_1 - \tfrac{1}{2}\Delta_2 + V_1(x_1) + V_2(x_2) + V_{12}(x_1 - x_2)$$

and $C_1 = \{0, 1\}, C_2 = \{2\}$ so that $R = x_2$; $\zeta = x_1$. We suppose that

$$(H\varphi)(x_1, x_2) = E\varphi(x_1, x_2)$$

and that

$$(H_1\eta)(x_1) = \Sigma\eta(x_1)$$

with $H_1 = -\frac{1}{2}\Delta_1 + V_1(x_1)$. E and Σ are supposed to be discrete ground states so that $\varphi > 0$, $\eta > 0$ and

$$\Sigma < \Sigma' = \inf \operatorname{spec}\left(H_1 \restriction \{\eta\}^{\perp}\right). \tag{3.1}$$

We suppose that for $\alpha = 1, 2$ or 12, we have

$$V_\alpha(y) = 0 \qquad \text{if } |y| > R_0 \tag{3.2}$$

for some fixed R_0 and each $V_\alpha \in L^\infty$. We also suppose regularity, so by Theorem 2.3, we have that

$$\int \eta(x_1)\varphi(x_1, x_2)\, dx_1 \geq C_\delta e^{-\delta|x_2|}\left[\int |\varphi(x_1, x_2)|^2\, dx_1\right]^{1/2}. \tag{3.3}$$

Now we want to study $\varphi(x_1, x_2)$ as we vary x_1 in the region $|x_1| < R_1$ and take $|x_2| \to \infty$. We will use the Feynman–Kac formula (2.8), which now reads

$$\varphi(x_1, x_2) = E\left(\exp\left(+\int_0^t (E - V)(x_1 + b_1(s), x_2 + b_2(s))\, ds\right)\right.$$

$$\left. \times \varphi(x_1 + b_1(t), x_2 + b_2(t)) \right), \tag{3.4}$$

where b_1 and b_2 are two independent ν-dimensional Brownian motions.

The strategy of the proof will be the following: in (3.4), we will take the $t = \epsilon|x_2|$ with ϵ very small. Since ϵ is small, and $|x_2| \to \infty$ particle two does not have a chance to get near either particle zero or one, so we can replace V by V_1 (see Lemma 3.1), that is,

$$\varphi(x_1, x_2) \cong \left(e^{-t(H_1 + H_{02} - E)}\varphi\right)(x_1, x_2)$$

(with $H_{02} = -\frac{1}{2}\Delta_2$) for $t = \epsilon|x_2|$. Since $|x_2| \to \infty$, the effect of e^{-tH_1} will be to project onto η; more precisely (see Lemma 3.2)

$$e^{-t(H_1 - \Sigma)}g = (\eta, g)\eta + O(e^{-t(\Sigma' - \Sigma)})\|g\|_2.$$

Equation (3.3) will enter in, showing that for $g = \varphi(\cdot, x_2)$, we can estimate $\|g\|_2$ by (η, g).

We begin the actual proof by noting that if we take t small enough, then $V = V_1 + V_2 + V_{12}$ in (3.4) can be replaced by V_1. We define

$$\psi(x_1, x_2; t) = E\left(\exp\left(+\int_0^t (E - V_1)(x_1 + b_1(s))\,ds\right)\right.$$
$$\left.\varphi(x_1 + b_1(t), x_2 + b_2(t))\right). \tag{3.5}$$

LEMMA 3.1. *For some $\epsilon, \alpha > 0$, we have that*

$$|\psi(x_1, x_2; t) - \varphi(x_1, x_2)| \leq Ce^{-\alpha|x_2|}\varphi(x_1, x_2) \tag{3.6}$$

as $|x_2| \to \infty$ uniformly in $0 < t \leq \epsilon|x_2|$ and $|x_1| < R_1$.

Proof. φ and ψ are integrals of integrands which only differ on paths $(b_1(s), b_2(s))$ for which either $|x_2 + b_2(s)| \leq R_0$ or $|x_1 + b_1(s) - x_2 - b_2(s)| \leq R_0$ for some s in $(0, t)$. Since the integrands are uniformly bounded by Ce^{at} for some fixed a, C (since $\varphi \in L^\infty$ [8] and we suppose that $V_\alpha \in L^\infty$), we see that

$$\begin{aligned}|\psi - \varphi| \leq \big[&\operatorname{Prob}(|x_2 + b_2(s)| \leq R_0) \\ &+ \operatorname{Prob}(|x_1 + b_1(s) - x_2 - b_2(s)| \\ &\leq R_0)\big]Ce^{at}.\end{aligned}$$

It is a standard estimate [8] that

$$\operatorname{Prob}(|b(s)| \geq A \qquad \text{for some } s \in [0, t]) \leq C_1 e^{-DA^2/t}.$$

Thus, for $|x_2| \geq 2R_0, 2R_0 + R$, and $|x_1| < R$, we find that

$$|\psi - \varphi| \leq C'e^{at}e^{-D'|x_2|^2/t}.$$

By (2.1), $|\varphi(x_1, x_2)| \geq Ce^{-b|x_2|}$ in the region in question. From these facts, (3.6) follows immediately. □

LEMMA 3.2. *For all $t \geq 1$ and functions f of x_1, we have that*

$$|(e^{-tH_1}f)(x_1) - (\eta, f)e^{-t\Sigma}\eta(x_1)| \leq Ce^{-t\Sigma'}\|f\|_2$$

with C a fixed constant independent of t and f.

Proof. Let P be the projection onto the orthogonal complement of $\{\eta\}$. Note that e^{-tH_1} is bounded from L^2 to L^∞ [2, 8] so that

$$\begin{aligned}\|e^{-tH_1}Pf\|_\infty &\leq \|e^{-H_1}\|_{L^2\to L^\infty}\|e^{-(t-1)H_1}Pf\|_2\\ &\leq \|e^{-H_1}\|_{L^2\to L^\infty}e^{-(t-1)\Sigma'}\|Pf\|_2\\ &\leq Ce^{-t\Sigma'}\|f\|_2\end{aligned}$$

since $e^{-tH_1}Pf = e^{-tH_1}f - (\eta,f)e^{-t\Sigma}\eta$, the lemma is proven. □

Now let

$$C(x_2,t) = E_{b_2}\left(\left[\int \eta(x_1)\varphi(x_1,x_2+b_2(t))\,dx_1\right]\right). \tag{3.7}$$

LEMMA 3.3. *For some fixed* γ, *smaller than the* ϵ *of Lemma* 3.1, *and* $\beta > 0$, *we have that* (*for* d *a fixed constant*)

$$\begin{aligned}|\psi(x_1,x_2;\gamma|x_2|) &- C(x_2,\gamma|x_2|)e^{-\gamma|x_2|(\Sigma-E)}\eta(x_1)|\\ &\leq dC(x_2,\gamma|x_2|)e^{-\gamma|x_2|(\Sigma-E)}e^{-\beta|x_2|}\end{aligned} \tag{3.8}$$

as $|x_2|\to\infty$, *uniformly in* $|x_1| < R_1$.

Proof. We begin by noting that by the Feynman–Kac formula for e^{-tH_1}, we have that

$$\psi(x_1,x_2;t) = E_{b_2}\left(\left(e^{-t(H_1-E)}\varphi_{x_2+b_2(t)}\right)(x_1)\right)$$

with $\varphi_y(x) = \varphi(x,y)$ as usual. By definition (3.7) we have that

$$C_2(x_2,t)e^{-t(\Sigma-E)}\eta(x_1) = E_{b_2}\left(e^{-t(\Sigma-E)}(\eta,\varphi_{x_2+b_2(t)})\eta(x_1)\right).$$

Thus, by Lemma 3.2, we have that

$$(\text{LHS of }(3.8)) \leq Ce^{-\gamma|x_2|(\Sigma'-E)}E_{b_2}\left(\|\varphi_{x_2+b_2(t)}\|\right).$$

By (3.3), for any δ

$$\begin{aligned}E_{b_2}\left(\|\varphi_{x_2+b(t)}\|\right) &\leq C_\delta E_{b_2}\left(e^{\delta|x_2+b_2(t)|}(\eta,\varphi_{x_2+b_2(t)})\right)\\ &\leq 2C_\delta E_{b_2}(\eta,\varphi_{x_2+b_2(t)})e^{2\delta|x_2|}\end{aligned}$$

since for γ small, we can be sure that $|b_2(t)| \leq |x_2|$ with overwhelming probability (the error from paths with $|b_2(t)| \geq |x_2|$ can easily be controlled by the fact that C_δ has been replaced by $2C_\delta$). As a result, (3.8) holds with

$$\beta = \gamma(\Sigma' - \Sigma) - 2\delta$$

and

$$d = 2C_\delta.$$

Since δ can be chosen arbitrarily small after picking γ, we can be sure that $\beta > 0$. $\square$

Putting together the estimates of the last three lemmas, we find that for $|x_1| < R_1$

$$\left\{\left[C(x_2, \gamma|x_2|)e^{-\gamma|x_2|(\Sigma - E)}\right]^{-1}\varphi(x_1, x_2) - \eta(x_1)\right\} \leq De^{-\mu|x_2|}$$

for μ large from which (1.2) immediately follows.

In the next section, we will state the precise result in more formal terms. Here we want to note the changes needed for more general N-body systems: Introduce the inner product, $(x,y) = \Sigma m_i x_i y_i$ on points $x = (x_1, \dots, x_N)$ and $y = (y_1, \dots, y_N)$ in $R^{N\nu}$. Let $\omega(t)$ be an $R^{N\nu}$-valued Gaussian process with covariance ($i = 1, \dots, N$; $a = 1, \dots, \nu$)

$$E\big(\omega_{ia}(t)\omega_{jb}(s)\big) = \delta_{ij}\delta_{ab}(m_i)^{-1}\min(t,s).$$

Let π be the orthogonal projection onto the plane $\Sigma m_i x_i = 0$ in the inner product introduced above and let $q(t) = \pi[\omega(t)]$. The Feynman–Kac formula reads

$$\varphi(x) = e^{tE}E\left(\exp\left[-\int_0^t \sum_{i<j} V_{ij}\big(q_i(s) - q_j(s)\big)\,ds\right]\varphi(x_i + q_i(t))\right).$$

We pick a two-cluster partition, D and coordinates (R_D, ζ_D). As before we keep $|\zeta_D|$ bounded and $|R_D| \to \infty$. We define $\psi(x;t)$ by the above Feynman–Kac formula but with all terms V_{ij} with $i \in C_1$, $j \in C_2$ or $i \in C_2, j \in C_1$ replaced by zero. Since $[q_i(s) - q_j(s)]$ is a Gaussian process with covariance $\delta_{ab}[(m_i)^{-1} + (m_j)^{-1}]\min(t,s)$, Lemma 3.1 goes through without any significant change. Lemma 3.2 now reads that for functions of ζ_D

$$|(e^{-t[H(C_1)+H(C_2)]}f)(\zeta_D) - (\eta, f)e^{-t\Sigma}\eta(\zeta_D)| \leq Ce^{-t\Sigma'}\|f\|_2$$

and is proven in just the same way. Finally, Lemma 3.3 goes through easily if we note that (ζ, R) are orthogonal coordinates in the above inner product, so that if q_ζ, q_R are the ζ and R components of q, then q_ζ and q_R are independent processes.

4. Asymptotics of the Ratio: General Potentials

Here we want to consider general potentials V_{ij} obeying

$$\int_{|y|<R_0} |V_{ij}(y)|^P d^\nu y < \infty \tag{4.1}$$

for some $P > \nu/2$ and some R_0. For $|y| > R_0$ we will suppose one of the following:

$$|V_{ij}(y)| \leq Ce^{-a|y|} \tag{4.2}$$

for some $a > 0$ or

$$|V_{ij}(y)| \leq D(1 + |y|)^{-\alpha} \tag{4.3}$$

for some $\alpha \geq 1$. The main result of this paper is:

THEOREM 4.1. *Let H be the Hamiltonian of an N-body system with potentials obeying* (4.1) *and either* (4.2) *or* (4.3). *Let D be a regular partition into two clusters C_1, C_2 with associated coordinates (ζ_D, R_D). Let H have a normalized ground state φ and suppose that $H(C_1) + H(C_2)$ have a discrete normalized ground state η. Then* (1.2) *holds and the convergence is uniform as ζ, ζ' run through compact subsets. If* (4.2) *holds, the errors are $O(e^{-\mu|R|})$ for some $\mu > 0$. If* (4.3) *holds, the errors are $o(R^{-(\alpha-1)})$.*

Remarks. 1. It is likely, one could replace pointwise hypotheses like (4.2), (4.3) by hypotheses on an average of $|V_{ij}(y)|^P$, but as (4.2), (4.3) hold in interesting cases, we have not tried to implement this improvement.

2. If (as happens in the atomic case) one has

$$|V_{ij}(y) - V_{ij}(z)| \leq C|y - z|(1 + R)^{-\alpha-1}$$

for $|y|, |z| > R > R_0$, then it might be possible to replace $o(R^{-(\alpha-1)})$ by $o(R^{-\alpha})$. This is because, rather than replace $V_{ij}(x_i + q_i(t) - x_j + q_j(t))$ by zero, we try to replace it by some quantity which is nonzero but independent of the ζ_D component of x.

Proof. We need only follow the proof in Section 3. The only change needed (if we use the N-body ideas described at the end of that section) is in the statement and proof of Lemma 3.1. Rather, (3.6) remains unchanged if (4.2) holds and $e^{-\alpha|x_2|}$ is replaced by $\epsilon D'(1 + \frac{1}{2}|x_2|)^{-(\alpha)}|x_2|$ if (4.3) holds. Given this changed lemma, the remaining proof is unchanged; the errors introduced in Lemma 3.3 are $o(e^{-\delta|x_2|})$ with constants diverging as $\epsilon\downarrow 0$.

The changed lemma requires some modifications in its proof: since V_{ij} is not supposed bounded, we cannot estimate

$$E\left(\exp\left(-\int_0^t V_{ij}\right);|q_i(s)-q_j(s)|\geq \tfrac{1}{2}|x_i-x_j|\right)$$

by

$$e^{t\|V_{ij}\|_\infty}\operatorname{Prob}\left(|q_i(s)-q_j(s)|\geq \tfrac{1}{2}|x_i-x_j|\right).$$

But, using the Schwartz inequality, we can bound it by

$$\left[E\left(\exp\left(-2\int_0^t V_{ij}\right)\right)\right]^{1/2}\operatorname{Prob}\left(|q_i(s)-q_j(s)|\geq |x_i-x_j|\right)^{1/2},$$

which is just as good, since the first expectation is $O(e^{at})$ [2, 8].

The main change in the proof involves how we control the expectation once we determine that the contributions with $|q_i(s)-q_j(s)|\leq \frac{1}{2}|x_i-x_j|$ are all that matter. The point is that modulo the contributions when this condition fails, φ and ψ are expectations of the form

$$\varphi = E(F),$$
$$\psi = E(Fe^{G}),$$

where $|G|\leq Ct(1+\frac{1}{2}|x_i-x_j|)^{-\alpha}\equiv\gamma$. Now we use

$$\begin{aligned}|\varphi-\psi| &= |E(F(e^{G}-1))|\\ &\leq |E(F)|[e^{\gamma}-1]\end{aligned}$$

since $F\geq 0$. This yields the required estimates. □

5. Absolute Asymptotics

In the previous two sections, we showed that for $\varphi(\zeta,R)$, and $\eta(\zeta)$ suitable ground states we have

$$c(R)^{-1}\varphi(\zeta,R)\to\eta(\zeta) \tag{5.1}$$

as $R\to\infty$, ζ fixed. If the potentials have compact support, then the error is $o(e^{-\mu|R|})$. This determines $c(R)$ uniquely up to errors of order $e^{-\mu|R|}$. In this section, we will examine two natural properties of $c(R)$; namely is it true that

$$c(R) = \int \eta(\zeta)\varphi(\zeta, R)\, d\zeta \tag{5.2}$$

and is it true that

$$c(R) = ce^{-KR}|R|^{-(\nu-1)/2}(1 + \text{small error}) \tag{5.3}$$

with K given by

$$\Sigma - E = \tfrac{1}{2}K^2\big(M(C_1)^{-1} + M(C_2)^{-1}\big).$$

The system (5.1), (5.2) is just the original conjecture of Hoffman-Ostenhof and Morgan. For potentials of compact support, we will prove both (5.2) and (5.3) in this section for regular D. As in Section 3, we will first consider the special three-body case with $m_0 = \infty$, $m_1 = m_2 = 1$ and then indicate the general case.

THEOREM 5.1. *For some fixed small σ, and fixed function $c(x_2)$ we have that*

$$|\varphi(x_1, x_2) - c(x_2)\eta(x_1)| \le De^{-[\rho(0,x_2)+\alpha|x_2|]} \tag{5.4}$$

for some $\alpha > 0$ and all x_1, x_2 with $|x_1| < \sigma|x_2|$.

Proof. We follow the proof of Section 3. Since $|x_1 - x_2|$ and $|x_2|$ are both large, Lemma 3.1 will hold with errors of the order of the right side of (5.4). Using Lemma 5.2, the errors in replacing $\psi(x_1, x_2, \gamma|x_2|)$ by $c(x_2)\eta(x_1)$ are the order of $e^{-(\Sigma'-\Sigma)\gamma|x_2|}\|\varphi_{x_2}(\cdot)\|_2$. □

Next we note that in the Appendix we show that for regular D,

$$\rho(R, \zeta = 0) = \sqrt{2\mu(\Sigma_D - E)}\,|R| \tag{5.5a}$$

with μ the reduced mass of the two clusters in D. In particular in the case at hand

$$\rho(x_1 = 0, x_2) = \sqrt{2(\Sigma - E)}\,|x_2|. \tag{5.5b}$$

THEOREM 5.2. *In (5.4), the function $c(x_2)$ can be replaced by*

$$\tilde{c}(x_2) = \int \eta(x_1)\varphi(x_1, x_2)\, dx_1. \tag{5.6}$$

Proof. By (2.1) and regularity, $\varphi(x_1, x_2) \le C_\delta e^{-\rho(0,x_2)+\delta|x_2|}$ and $|\eta(x_1)| \le De^{-\alpha'|x_1|}$ for some α'. Thus

$$\int_{|x_1|>\sigma|x_2|} \eta(x_1)\varphi(x_1, x_2)\,dx_1 \le Ce^{-\rho(0,x_2)-\alpha'\sigma|x_2|/2}.$$

By (5.4), and the fact that $\eta \in L^1$ we therefore have that

$$|\tilde{c}(x_2) - c(x_2)| \le D\exp\left(-\left[\tilde{\alpha} + \sqrt{2(\Sigma - E)}\,\right]|x_2|\right)$$

with $\tilde{\alpha} = \min(\alpha, \frac{1}{2}\alpha'\sigma)$. But, by (2.1) and (5.5):

$$\tilde{c}(x_2) \ge D'\exp\left(-\left[\tfrac{1}{2}\tilde{\alpha} + \sqrt{2(\Sigma - E)}\,\right]|x_2|\right)$$

so that $|c(x_2)/\tilde{c}(x_2) - 1| = O(e^{-\tilde{\alpha}|x_2|/2})$. Thus (5.4) holds with c replaced by $\tilde{c}$ with a changed value of α. □

LEMMA 5.3. *Suppose that* (5.5) *holds and let* $\tilde{c}$ *be given by* (5.6). *Then* $\tilde{c}$ *obeys*:

$$-\tfrac{1}{2}(\Delta\tilde{c})(y) = (E - \Sigma)\tilde{c}(y) + Q(y)\tilde{c}(y) \tag{5.7}$$

with

$$|Q(y)| \le De^{-\nu|y|} \tag{5.8}$$

for some $\nu > 0$.

Proof. Since $[-\frac{1}{2}\Delta_{x_1} + V_1(x_1)]\eta(x_1) = \Sigma\eta(x_1)$ we have that

$$\begin{aligned} -\Sigma\tilde{c}(x_2) &= -\int \varphi(x_1, x_2)\left[-\tfrac{1}{2}\Delta_{x_1} + V_1(x_1)\right]\eta(x_1)\,dx_1 \\ &= \int (-H\varphi)(x_1, x_2)\eta(x_1)\,dx_1 + \int\left(-\tfrac{1}{2}\Delta_{x_2} + V_2 + V_{12}\right)\varphi\eta\,dx_1 \\ &= -\tfrac{1}{2}\Delta_{x_2}\tilde{c}(x_2) + Q(x_2)\tilde{c}(x_2) - E\tilde{c}(x_2), \end{aligned}$$

where

$$\begin{aligned} Q(x_2) &= V_2(x_2) + \tilde{Q}(x_2), \\ \tilde{Q}(x_2) &= \tilde{c}(x_2)^{-1}\int V_{12}(x_1 - x_2)\varphi(x_1, x_2)\eta(x_1)\,dx_1. \end{aligned}$$

Since $|\eta(x_1)| \le Ce^{-2\nu|x_1|}$ for some $\nu > 0$ and V_{12} has compact support

$$|\tilde{Q}(x_2)| \le Ce^{-2\nu|x_2|}\tilde{c}(x_2)^{-1}\int \varphi(x_1, x_2)\,dx_1.$$

But, by the arguments in the proof of Theorem 2.3

$$\int \varphi(x_1, x_2)\, dx_1 \leq D \exp\left(+ \left[\tfrac{1}{2}\nu - \sqrt{2(E - \Sigma)}\, \right] |x_2| \right)$$

and, by (2.1),

$$\tilde{c}(x_2)^{-1} \leq D' \exp\left(\left[\tfrac{1}{2}\nu + \sqrt{2(E - \Sigma)}\, \right] |x_2| \right). \qquad \square$$

LEMMA 5.4. *Let Q obey* (5.8) *and let*

$$-\tfrac{1}{2}\Delta f = -\tfrac{1}{2}k^2 f - Q(y) f$$

with $k > 0$ and $f \geq 0$, $f \not\equiv 0$, and $f \in L^2$. Then, for some $d \neq 0$;

$$f(y) = d e^{-k|y|}\left[|y|^{-(\nu-1)/2} \right]\left(1 + o(|y|^{-1})\right]. \tag{5.9}$$

If Q is rotationally symmetric, then $e^{-k|y|}|y|^{-(\nu-1)/2}$ can be replaced by the Bessel function, $x^{-\nu/2+1}K_{\nu/2-1}(kx)$, and $o(|y|^{-1})$ by $o(e^{-\lambda|y|})$.

Remarks. 1. By taking $Q(y) = V(y - a)$ with a fixed and V rotationally invariant, we see that $o(|y|^{-1})$ in (5.9) cannot be improved in general.

2. If $\nu = 3$, the Bessel function is exactly $(4\pi|x|)^{-1}\exp(-k|x|)$.

Proof. Let $G(x - y)$ be the fundamental solution of $-\frac{1}{2}\Delta + \frac{1}{2}k^2$. Then

$$f(x) = -\int G(x - y) Q(y) f(y). \tag{5.10}$$

By standard arguments (e.g., [7, Sect. XIII.13]), $|f(y)| \leq C_\delta e^{-(k-\delta)(y)}$. Thus, by (5.8) and the asymptotics of G:

$$f(x) = d e^{-k|y|}\left[|y|^{-(\nu-1)/2} \right] + o\left[e^{-k|y|}(y)^{-(\nu+1)/2} \right].$$

All that remains is that we prove that $d \neq 0$ for the general case. But

$$d = -(\text{const}) \int Q(y) f(y)\, dy$$

and by the fundamental equation

$$-\int Q(y) f(y)\, dy = \lim_{g \to 1, g \in C_0^\infty} -\int Q(y) f(y) g(y)\, dy$$

$$= \lim_{g \to 1, g \in C_0^\infty} \int f(y)\left(-\tfrac{1}{2}\Delta + \tfrac{1}{2}k^2\right) g(y)\, dy = \tfrac{1}{2}k^2 \int f\, dy \neq 0.$$

For the case with Q rotationally symmetric, we can use standard ODE methods. For example, the case $\nu = 3$ is described in Section XI.8 of [6, see especially (130a)]. □

Combining the above, we obtain the special case of the following N-body result whose proof is identical:

THEOREM 5.5. *Let H be the Hamiltonian of an N-body system with potentials of compact support. Let D be a regular breakup so that, in particular (see the Appendix)*

$$\rho(R, \zeta = 0) = K|R|$$

with $K^2/2\mu = \Sigma - E$ with μ the reduced mass of the two clusters and $E = \inf spec(H), \Sigma = \inf spec(H(C_1) + H(C_2)$. Suppose that E, Σ are discrete eigenvalues of their respective Hamiltonians with normalized ground states φ, η. Then

$$\varphi(\zeta, R)\left[\int [\varphi(\zeta, R)]^2 d\zeta\right]^{-1/2} \to \eta(\zeta)$$

as $R \to \infty$ both in $L^2(d\zeta)$ and uniformly on compacts. Moreover,

$$\varphi(\zeta, R)\left[e^{-KR}R^{-(\nu-1)/2}\eta(\zeta)\right]^{-1} = c\left(1 + O(R^{-1})\right)$$

as $R \to \infty$ for some $c \neq 0$ uniformly in $|\zeta| \leq R_1$. If all potentials are rotationally symmetric, then

$$\varphi(\zeta, R) = c\eta(\zeta)K_{\nu/2-1}(KR)R^{-\nu/2+1}\left(1 + O(e^{-\lambda R})\right)$$

as $R \to \infty$ uniformly in $|\zeta| \leq R_1$.

APPENDIX: SOME GEOMETRY OF THE AGMON METRIC

Fix a two cluster breakup, $D = \{C_1, C_2\}$ and consider two conditions in terms of the associated coordinates, (R, ζ):

(1) D is regular, i.e., if R is fixed $\rho(R, \zeta)$ has its minimum at $\zeta = 0$.

(2) The Agmon geodesic from $(R_0, \zeta = 0)$ to $(0, 0)$ lies in the plane $\{(R, \zeta) | \zeta = 0)\}$.

Here we want to demonstrate that (1) implies (2) but that (2) does not imply (1).

EXAMPLE ((2) holds; (1) does not). *We will take an extreme case where $E = \Sigma \neq \Sigma_D$ and some particles have infinite mass. By a continuity argument it is easy to arrange $m_i < \infty, E < \Sigma$. There will be three particles, with*

$m_0 = \infty$, $m_1 = m_2 = \frac{1}{2}$, $E = -1$ and the thresholds are -1 for the decompositions (01), (2) *and* (02), (1) *but only* -0.75 *for* (0) (12). *Thus segments in the planes $x_1 = 0$ or $x_2 = 0$ have zero length, segments in the plane $x_1 = x_2$ have length which is $\frac{1}{2}$ their "Euclidean length,"* $\frac{1}{2} = [(\delta x_1)^2 + (\delta x_2)^2]^{1/2}$, ($\frac{1}{2} = \sqrt{1 - 0.75}$) *and segments in the rest of space have Euclidean length. Take $D = (0)\ (12)$, so $\zeta = x_1 - x_2$; $R = \frac{1}{2}(x_1 + x_2)$. Then with R fixed, $\rho(R, \zeta)$ is minimized at the points $x_1 = 0$ or $x_2 = 0$ (i.e., $\zeta = \pm 2R$). But the geodesic from $(R, \zeta = 0)$ to $(0,0)$ is on the plane $\zeta = 0$ since this has length $\frac{1}{2}(\sqrt{2}\ R)$. ($\sqrt{2}$ is $\sqrt{2\mu}$ with $\mu = 1$ the reduced mass of ∞ and $\frac{1}{2} + \frac{1}{2}$, i.e., $x_1^2 + x_2^2 = 2R^2 + \frac{1}{2}\zeta^2$.) The competing path is a straight line from $(x_1 = R, x_2 = R)$ to $(x_1 = R, x_2 = 0)$ and then to $(0,0)$ has length $R > (\sqrt{2}/2)R$. Incidentally, if -0.75 is replaced by -0.5, then this provides an example with nonunique geodesic (see also* [3]).

In the other direction, we have:

THEOREM A.1. *If D is regular,* (2) *holds; in fact, every other path other than the one $((1 - s)R_0, 0)$ has strictly larger length. In particular, if D is regular, then*

$$\rho(R, \zeta = 0) = \sqrt{2(\Sigma_D - E)\mu}\ |R|$$

with μ the reduced mass of the two clusters.

Proof. We consider a path $(R(s), \zeta(s))$ from $(R_0, 0)$ to $(0,0)$ with $\zeta(s) \neq 0$ for some s and prove that it can be strictly shortened in length. Consider some s_0 with $\zeta(s_0) \neq 0$ and let $s_1 = \sup\{s < s_0 | \zeta(s) = 0\}$. Obviously $R(s_1) \neq 0$ (otherwise, consider instead the path up to s_1) so for some $s_2 \in (s_1, s_0)$, we can be sure that the decomposition $D'(s)$ determined by $(R(s), \zeta(s))$ obeys: $D'(s)$ refines D for all $s \in (s_1, s_2)$.

Thus, the length of the segment of path from s_1 to s_2 is at least $\sqrt{\Sigma_D - E}\ (\mu[R(s_1) - R(s_2)]^2 + l(\zeta(s_2))^2)^{1/2}$ with $l(\zeta(s_2))$ the length of $\zeta(s_2)$ in the mass weighted Euclidean metric. This is because every weight $\sqrt{\Sigma_{D'(s)} - E}$ entering obeys $\Sigma_{D'(s)} \geq \Sigma_D$. The length of the segment after s_2 is at least $\rho(R(s_2), \zeta(s_2))$, so the length from s_1 to the end is at least

$$\sqrt{\Sigma_D - E}\left(2\mu[R(s_1) - R(s_2)]^2 + 2l(\zeta(s_2))^2\right)^{1/2} + \rho(R(s_2), 0)$$

since $\rho(R(s_2), \zeta(s_2)) \geq \rho(R(s_2), 0)$ by regularity. But the path from $(R(s_1), \zeta(s_1) = 0)$ to $(0,0)$ which is initially a straight line to $(R(s_2), 0)$ and then a geodesic from $(R(s_2), 0)$ to $(0,0)$ has length

$$\sqrt{\Sigma_D - E}\left(2\mu(R(s_1) - R(s_0))^2\right)^{1/2} + \rho(R(s_2), 0)$$

which is strictly smaller. □

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