ON THE ROLE OF PAIR EXCITATION IN THE EVOLUTION OF CONDENSATES

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Abstract. Joint work with **M. Machedon and D. Margetis.** In the present talk I would like to consider certain aspects of the evolution of N indistinguishable quantum particles (Bosons), for N large but finite under binary interactions. The evolution of the condensate is described by a mean filed which satisfies a Hartree type evolution. We consider a correction which takes into account the evolution of coherent pairs (pair excitations) coupled to the mean field and we compare the exact with the approximate dynamics.

1. The Classical picture

• Consider N quantum particles with wavefunction $\psi(t, x_1 x_2 \ldots x_N)$ (assume that $h = 2m = 1$) the particles are non-relativistic. The evolution of this system is described by the PDE

$$\frac{1}{i}\partial_t \psi = H_N \psi \quad \text{with some data} \quad \psi(t=0) := \psi_0 \tag{1}$$

The N-body Hamiltonian is

$$H_N := \sum_{a=1}^{N} -\Delta_a + \frac{1}{2N}\sum_{a \neq b} N^{3\beta} v(N^{\beta}|x_a - x_b|) \quad \text{where} \quad 0 \leq \beta \leq 1 \tag{2}$$

We take into account only two body interactions. Δ_a is the Laplacian in the x_a coordinates and for later use set:

$$v^N := N^{3\beta} v(N^{\beta}\cdot) \qquad \text{where} \quad 0 \leq \beta \leq 1 \ .$$

One can think of this as the description of a dilute quantum gas. The solution of the equation above can be written in an abstract form

$$\psi(t) = e^{itH_N}\psi(0) \ ,$$

but this formula is not very informative since we are interested in $N >> 1$, typicaly N is of the order of 10^4 to 10^{23}.

• What is really important is the fact that we are actually interested in the evolution of ψ starting from special initial data of the form, **(factorized)**

$$\psi_0(x_1, x_2 \dots x_N) := \prod_a \phi_0(x_a) \quad ; \quad \text{tensor product} \tag{3}$$

i.e. the initial data are a tensor product of a single wave function $\phi_0(x)$. (All particles are in the same state ϕ.) Why are we interested in this type of question?

2. BEC and background information

Bosons mean that the wave-function is invariant under particle permutations,

$$\psi(t, x_{\sigma(1)}, x_{\sigma(2)}, \dots x_{\sigma(N)}) = \psi(t, x_1, x_2, \dots x_N) \quad ; \quad \sigma \text{ permutation}$$

Here is a very brief outline on Bose-Einstein condensates.The references are on theoretical (and or) Mathematical work.

• **The static problem :** (for example in the presence of a trap, the particles interact even at zero temperature) Original idea of Bose with Einstein considering the Statistics of a large number of (noninteracting) Quantum particles. A condensate is formed below a temperature that depends on the density of the gas. The question is to characterize the "ground state". Early work by F. Dyson and Bogoliubov, also Lee, Huang and Yang, more recent : Rigorous treatment in fundamental work(s) by : Lieb, Seiringer and Yngvanson.

• **The dynamic problem :** (for example, remove the trap and follow evolution) The point is that we start from data that are in some sense approximately factorized. Framework by Spohn; and rigorous treatment in the fundamental work : Elgart and Erdös, Schlein, H. T. Yau in a series of papers. This generated further work see Klainerman, Machedon... Kirkpatrick, Staffilani, Schlein... Chen, Pavlovich... X. Chen etc.

• **Outline of relevant results :** Form the two point marginal,

$$\gamma_{N,1}(t, x_1, x_1') := \int dy_2 \dots dy_N \left\{ \overline{\psi}(t, x_1', y_2 \dots y_N)\psi(t, x_1, y_2 \dots y_N) \right\} .$$

Condensate means that, (Penrose and Onsager, dominant eigenvalue of γ_N)

$$\|\gamma_{N,1} - \phi \otimes \overline{\phi}\|_{HS} \to 0 \quad \text{as} \quad N \to \infty , \tag{4}$$

where HS indicates the Hilbert-Schmidt norm. Thus ϕ describes the state of a "typical" particle and we can ask how the typical particle evolves. The evolution of the condensate wave-function $\phi(t,x)$ is described by a nonlinear equation, (the answer depends on the strength of interactions)

$$-i\dot{\phi} - \Delta\phi + g_\beta\big(|\phi|^2\big)\phi = 0 \quad \text{and} \quad \phi(0) = \phi_0 \ .$$

The above is a nonlinear Scrödinger type equation where the nonlinearity is,

$$\begin{aligned}
g_0(|\phi|^2) &= v * |\phi|^2 && \text{Hartree evolution} \\
g_\beta(|\phi|^2) &= \big(\int v\big)|\phi|^2 \quad ; && 0 < \beta < 1 \quad \text{NLS} \\
g_1(|\phi|^2) &= 8\pi a|\phi|^2 && \text{Gross Pitaevskii}
\end{aligned}$$

• **Scattering length :** In the last case a is the scattering length of the two body interaction via the potential v i.e. $-\Delta w + (1/2)vw = 0$ with $\lim_{x\to\infty} w = 1$ and for $|x|$ large

$$w \approx 1 - \frac{a}{|x|} \qquad a \text{ is the scattering length.}$$

The case $\beta = 1$ is the critical scaling. Particles develop short length correlations which in the limit gives the modification in G-P . The problem is to explain how this happens... (see again Erdös, Schlein, H. T. Yau for the treatment of this problem) (also Lieb, Seringer for the static problem, different techniques). The point here is that one cannot see the emergence of scattering length via a naive factorized ansatz.

• **Estimates for N large finite :** Our motivation comes from (Rodnianski, Schlein), (Pioneering work by Hepp and Ginibre, Velo) (also Lee-Huang-Yang and T.T. Wu, different aspect) estimate of the type,

$$\|\gamma_{N,1} - \phi \otimes \overline{\phi}\|_{HS} \leq \frac{e^{ct}}{N} \quad \text{where } N \quad \text{is large finite.} \tag{5}$$

• **A note on the model :**The experiments, (see (Phillips) Anderson, Davis, Wieman, Mewes, Keterle et al) (1995) use alkali atoms. (these are complicated objects) Spin is crucial in trapping and cooling them. Particles behave approximately like Bosons only if the gas is dilute and the spin takes integer values (for example $s = -1, 0, 1$ corresponds to three different states i.e. a mixture of three gases). At shorter distances internal structure is important!

3. Second Quantization

There is another, complementary, way to look at the problem. The Fock space formalism

$$\mathbb{F} := \sum_n \oplus \mathbb{F}_n \quad \text{where} \quad \mathbb{F}_n := L^2_s(\mathbf{R}^{3n})$$

i.e. a state can be written as a collection,

$$\big|\psi\big\rangle := \big(\psi_0\ ,\ \psi_1\ ,\ \dots \psi_n\ \dots\big)$$

$$\psi_n(x_1 x_2 \dots x_n) \quad \text{a symmetric function of } n \text{ variables.}$$

• **Creation and anihilation (distribution valued) operators :**

$$a^*_x(\psi_{n-1}) := n^{-1/2} \sum_{a=1}^{n} \psi_{n-1}(x_1 \dots x_{a-1}, x_{a+1} \dots x_n)\delta(x - x_a)$$

$$a_x(\psi_{n+1}) := \sqrt{n+1}\psi_{n+1}([x], x_1 \dots x_n) \quad [x] \quad \text{means frozen .}$$

For state ϕ we construct unbounded operators

$$a^*_\phi := \int dx\, \{\phi(x) a^*_x\} \quad \text{and} \quad a_{\overline{\phi}} := \int dx\, \big\{\overline{\phi} a_x\big\}\ \text{, etc.}$$

By convention we use conjugate with anihilation operators.

• **Notation :** Write $a_a := a_{x_a}$, $a^*_a := a^*_{x_a}$ for $a = 1, 2 \dots$ and

$$\mathcal{Q}^*_{1,2} := a^*_1 a^*_2 \quad ; \quad \mathcal{Q}_{1,2} := a_1 a_2 \quad ; \quad \mathcal{D}_{1,2} := a^*_1 a_2$$

The Fock space Hamiltonian is,

$$\mathcal{H}_N := \int dx_1 dx_2 \big\{ -\Delta_1 \delta_{1-2} \mathcal{D}_{1,2} + (1/2N) V_{1-2} \mathcal{Q}^*_{1,2} \mathcal{Q}_{1,2} \big\} \tag{6}$$

and the evolution in Fock space is described by,

$$\frac{1}{i}\partial_t \big|\psi\big\rangle = \mathcal{H}_N \big|\psi\big\rangle \quad \text{with data} \quad \big|\psi(0)\big\rangle := \big|\psi_0\big\rangle \tag{7}$$

The vacuum state is

$$\big|0\big\rangle = (1, 0, 0 \dots) \quad \text{so that,} \quad a\big|0\big\rangle = 0\ .$$

• **Coherent states :** are created via,

$$\mathcal{A}(\phi) := \int dx\, \big\{ -\overline{\phi}(t,x) a_x + \phi(t,x) a^*_x \big\}$$

$$W_\phi := e^{-\sqrt{N}\mathcal{A}(\phi)} \quad \text{Weyl operators.}$$

indeed the N-th entry in Fock space is a tensor product

$$\big|\psi_{\text{coherent}}\big\rangle = e^{-\sqrt{N}\mathcal{A}(\phi(0))}\big|0\big\rangle = \Big(\dots\ c_N \prod_{a=1}^{N} \phi_0(x_a)\ \dots\Big)$$
$$\text{where} \quad c_N \approx N^{1/4} \ .$$

We want to compare the exact with the approximate dynamics,

$$\big|\psi_{\text{exact}}\big\rangle = e^{it\mathcal{H}_N} e^{-\sqrt{N}\mathcal{A}(\phi(0))}\big|0\big\rangle$$
$$\big|\psi_{\text{appr}}\big\rangle := e^{-\sqrt{N}\mathcal{A}(\phi(t))}\big|0\big\rangle$$

where $\phi(t)$ is to be determined. The number operator (counts the average number of particles) is

$$\mathcal{N} := \int dx_1 \left\{\mathcal{D}_{1,1}\right\} \quad \text{compute the observable}$$
$$\big\langle\psi\big|\mathcal{N}\big|\psi\big\rangle = N \quad \text{where} \quad \big|\psi\big\rangle = e^{-\sqrt{N}\mathcal{A}(\phi)}\big|0\big\rangle \quad \text{and } \|\phi\|^2 = 1 \ .$$

• **The reduced dynamics :** Follow the exact dynamics and come back using the approximate dynamics to form the reduced dynamics,

$$\big|\psi_{red}\big\rangle := e^{\sqrt{N}\mathcal{A}(\phi(t))} e^{it\mathcal{H}_N} e^{-\sqrt{N}\mathcal{A}(\phi(0))}\big|0\big\rangle \quad \text{where} \quad \big|\psi_{red}(0)\big\rangle = \big|0\big\rangle \ .$$

The reduced dynamics satisfies the evolution,

$$(1/i)\partial_t\big|\psi_{\text{red}}\big\rangle = \mathcal{H}_{\text{red}}\big|\psi_{\text{red}}\big\rangle \quad ; \quad \big|\psi_{red}(0)\big\rangle = \big|0\big\rangle \tag{8}$$

with the reduced Hamiltonian,

$$\mathcal{H}_{\text{red}} := i\left(\partial_t e^{\sqrt{N}\mathcal{A}}\right) e^{-\sqrt{N}\mathcal{A}} + e^{\sqrt{N}\mathcal{A}}\mathcal{H}_N e^{-\sqrt{N}\mathcal{A}}$$

A crucial fact is the formula,

$$e^{\mathcal{A}}\mathcal{H}e^{-\mathcal{A}} = \sum_{n=0}^{\infty} \frac{1}{n!}\text{ad}^n_{\mathcal{A}}(\mathcal{H})$$

where $\text{ad}^n_{\mathcal{A}}(\mathcal{H})$ means n commutations with respect to $\mathcal{A}$. $\mathcal{A}$ is a first order polynomial in (a, a^*) and if $\mathcal{P}_n$ is a polynomial of degree n then,

$$[\mathcal{A}, \mathcal{P}_n] = \mathcal{P}_{n-1}$$

i.e. commutation brings down the degree by one. This implies that we can compute explicitly,

$$\mathcal{H}_{\text{red}} = N\mu + N^{1/2}\mathcal{P}_1 + \mathcal{P}_2 + N^{-1/2}\mathcal{P}_3 + N^{-1}\mathcal{P}_4 \ . \tag{9}$$

As a matter of fact,

$$\mathcal{P}_1 = \int dx \left\{h(x)a^*_x + \overline{h}(x)a_x\right\} \quad ; \quad h := -i\phi_t - \Delta\phi + \left(v^N * |\phi|^2\right)\phi$$

The zeroth order term can be absorbed as a phase factor and it is natural to remove the $N^{1/2}$ term by setting $h = 0$ which gives the mean field dynamics. This is an explanation as to why the mean field emerges as an approximation of the exact dynamics. The nature of the approximation is not clear at this point. See Ginibre, Velo and more recently Rodnianski, Schlein.

4. The second order correction

This set up was recently used by Benedikter, de Oliveira, Schlein in the critical scaling (emergence of scattering length). Try an approximation of the form,

$$\big|\psi_{appr}\big\rangle := e^{-\sqrt{N}\mathcal{A}(\phi)} e^{-\mathcal{B}(k)}\big|0\big\rangle \qquad \text{where}$$
$$\mathcal{B}(k) := \int dx_1 dx_2 \left\{-k_{1,2}\mathcal{Q}^*_{1,2} + \overline{k}_{1,2}\mathcal{Q}_{1,2}\right\}$$

$k(t, x_1, x_2)$ kernel to be computed in a manner "consistent" with the N body dynamics. The idea is that $k(t, x_1, x_2)$ describes a pair of particles that left the condensate and evolve over a condensate background. We are interested in the dynamics of these **"pair excitations"**. The new reduced dynamics are described by

$$(1/i)\partial_t\big|\psi_{\mathrm{red}}\big\rangle = \mathcal{H}_{\mathrm{red}}\big|\psi_{\mathrm{red}}\big\rangle \quad ; \quad \big|\psi_{\mathrm{red}}(0)\big\rangle = \big|0\big\rangle \tag{10}$$

where the new reduced Hamiltonian is

$$\mathcal{H}_{\mathrm{red}} = \frac{1}{i}\big(\partial_t e^{\mathcal{B}}\big)e^{-\mathcal{B}} + e^{\mathcal{B}}\frac{1}{i}\big(\partial_t e^{\sqrt{N}\mathcal{A}}\big)e^{-\sqrt{N}\mathcal{A}}e^{-\mathcal{B}} + e^{\mathcal{B}}e^{\sqrt{N}\mathcal{A}}\mathcal{H}e^{-\sqrt{N}\mathcal{A}}e^{-\mathcal{B}}$$

Since we start from the vacuum, consider the difference $\big|\widetilde{\psi}\big\rangle := \big|\psi_{red}\big\rangle - \big|0\big\rangle$ which satisfies

$$\frac{1}{i}\partial_t\big|\widetilde{\psi}\big\rangle = \mathcal{H}_{\mathrm{red}}\big|\widetilde{\psi}\big\rangle + \mathcal{H}_{\mathrm{red}}\big|0\big\rangle$$

and do an energy estimate with $\mathcal{H}_{\mathrm{red}}\big|0\big\rangle$ as forcing...this means that we have to estimate $\mathcal{H}\big|0\big\rangle$ which has entries only in the two up to four slots in Fock space vectors. Our task is to compute $\mathcal{H}_{\mathrm{red}}$. The crucial observation is that the series

$$e^{\mathcal{B}}\mathcal{H}e^{-\mathcal{B}} = \sum_n \frac{1}{n!}\mathrm{ad}^n_{\mathcal{B}}(\mathcal{H})$$

exibits periodicity and therefore can be summed. There is a subtle connection between symplectic matrices and quadratic polynomials in creation and anihilation operators.

• **Lie Algebra Isomorphism :** Write,

$$\mathcal{A}_x^T := (a_x \ , \ a_x^*) \quad \text{and} \quad J := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad K_{1,2} := \begin{pmatrix} d_{1,2} & \overline{k}_{1,2} \\ l_{1,2} & -d_{2,1} \end{pmatrix}$$

Consider the map

$$\mathcal{H} : K \mapsto \mathcal{H}(K) \quad \text{via} \quad \mathcal{H}(K) := \big\langle \mathcal{A}_1^T \ \big| \ K_{1,2} \ \big| \ J\mathcal{A}_2 \big\rangle$$
$$\text{we have} \quad \big[\mathcal{H}(K), \mathcal{H}(L)\big] = \mathcal{H}\big([K,L]\big)$$

Weil, Segal-Shale, Bogoliubov in a restricted context. In our case we have

$$e^{\mathcal{B}} \mapsto \exp \begin{pmatrix} 0 & \overline{k} \\ k & 0 \end{pmatrix} = \begin{pmatrix} \mathrm{ch}(k) & \overline{\mathrm{sh}(k)} \\ \mathrm{sh}(k) & \overline{\mathrm{ch}(k)} \end{pmatrix}$$

where for example

$$\mathrm{sh}(k) = k + \frac{1}{3!} k \circ \overline{k} \circ k + \dots \quad \text{operator product}$$
$$(k \circ l)(x_1 x_2) := \int dy \, \{k(x_1, y) l(y, x_2)\} \quad \text{which means } k \circ l \neq l \circ k$$

• **New reduced dynamics :** Again the reduced Hamiltonian is a polynomial

$$\mathcal{H}_{\mathrm{red}} = N\mu + \sqrt{N}\mathcal{P}_1 + \mathcal{P}_2 + N^{-1/2}\mathcal{P}_3 + N^{-1}\mathcal{P}_3$$

The idea is to remove terms from $\mathcal{P}_2$ of the form $a^* a^*$, for this purpose it is crucial to look at

$$v^N_{1-2}\phi_1\phi_2 a_1^* a_2^* \qquad \text{call} \quad m^N_{1,2} := v^N_{1-2}\phi_1\phi_2 \quad \text{where } v^N := N^{3\beta} v(N^\beta \cdot)$$

this creates a pair at (x_1, x_2) and we would like to follow its evolution. Here is the idea. Form the following type of operator,

$$g_{1,2} := -\Delta_1 \delta_{1-2} + V_{1-2}\overline{\phi}_1\phi_2 + \big(V * |\phi|^2\big)\delta_{1-2} \ .$$

For a pair of functions $u(t, x_1, x_2)$ symmetric and $p(t, x_1, x_2)$ conjugate symmetric in (x_1, x_2) we consider the operators,

$$\mathbf{S}(u) := \frac{1}{i}\partial_t u + g^T \circ u + u \circ g \qquad \text{Schrodinger type,}$$
$$\mathbf{W}(p) := \frac{1}{i}\partial_t p + [g, p] \qquad \text{Wigner type.}$$

The evolution is expressed in terms of (new variables)

$$u := \mathrm{sh}(2k) \qquad \text{and} \qquad c := \mathrm{ch}(2k)$$

and it is a pair of linear equations:

$$\mathbf{S}(u) = m^N \circ c + \overline{c} \circ m^N \tag{11}$$

$$\mathbf{W}(\overline{c}) = m^N \circ \overline{u} - u \circ \overline{m}^N \ , \tag{12}$$

where $m^N(t, x_1, x_2) = N^{3\beta} v(N^\beta(x-y))\phi(t,x_1)\phi(t,x_2)$ acts as forcing (notice that $c = \delta + \text{l.o.t.}$).

• **Hartree dynamics :** Notice that if $\beta = 0$ the dynamics are independent of N which makes the problem easier.The following a-priory estimate

$$\|u(T)\|_{L^2} \leq \left(\int_0^T \|m\| dt + \|u(0)\| \right) e^{\int_0^T \|m\| dt}$$

tells us that we have to estimate

$$m_{1,2} := v_{1-2}\phi_1\phi_2 \quad \text{independent of } N$$

i.e. we want

$$\int_0^\infty \|m\|_{L^2} dt < \infty \ .$$

Once we have these ingredients in place we can estimate the forcing in

$$\frac{1}{i}\partial_t \big|\widetilde{\psi}\big\rangle = \mathcal{H}_{\text{red}}\big|\widetilde{\psi}\big\rangle + \mathcal{H}_{\text{red}}\big|0\big\rangle$$

and obtain,

$$\big\| \big|\psi_{exact}\big\rangle - \big|\psi_{appr}\big\rangle \big\|_{\mathbb{F}} \leq \frac{\sqrt{1+t}}{\sqrt{N}} \ . \tag{13}$$

• **Joint work with M. Machedon :** The case where $m^N(t, x_1, x_2) = N^{3\beta} v(N^\beta(x_1 - x_2))\phi(t, x_1)\phi(t, x_2$ is subtler. Now the dynamics depend on the number of particles and we can obtain an estimate of the form

$$\big\| \big|\psi_{exact}\big\rangle - \big|\psi_{appr}\big\rangle \big\|_{\mathbb{F}} \leq \frac{\log^4(1+t)\sqrt{1+t}}{N^{(1-3\beta)/2}} \tag{14}$$

which is meaningful for $\beta < 1/6$. Here is a technical but essential observation: The equation $\mathbf{S}(u) = m$ looks (in the limit $N \to \infty$) as $\mathbf{S}(u) = \phi^2\delta(x-y)$. The right hand side is not in any L^p space for $p > 1$ which means that Strichartz type estimates are not useful.

5. Recent progress

(Joint work with M. Machedon.) A new idea is that the system (condensate, pair excitations) can be derived through a general framework and a Lagrangian formulation. Namely we have a Lagrangian of the form,

$$\begin{aligned}
&\mu\big(\phi,\overline{\phi},u,\overline{u}\big) \qquad \text{from which we derive}\\
&\frac{\delta\mu}{\delta\overline{\phi}}=0 \qquad \text{and} \qquad \frac{\delta\mu}{\delta\overline{u}}=0 \quad \text{equations of motion}
\end{aligned}$$

This follows from the following general scheme: Observe that

$$\mathcal{H}_{\text{red}}\big|0\big\rangle=\big(X_0,X_1,X_2,X_3,X_4,0,\dots\big)$$

and form $\mu:=\int dt\{X_0\}$. Now

$$\begin{aligned}
\frac{\delta\mu}{\delta\overline{\phi}}&=0 \quad \text{implies} \quad X_1=0\\
\frac{\delta\mu}{\delta\overline{u}}&=0 \quad \text{implies} \quad X_2=0
\end{aligned}$$

This system conserves the total number of particles,

$$\text{number of particles}=N\|\phi\|^2+\|u\|^2$$

as well as an associated energy (the Lagrangian is translation invariant). Moreover the system is defocusing which implies that it is amenable to correlation (Morawetz type) estimates.

• **Minimal coupling model :** This simplified model captures the essential features,

$$\frac{1}{i}\partial_t\phi_1-\Delta\phi_1+\int dx_2\left\{v^N_{1-2}\big(\phi_1\phi_2+N^{-1}u_{1,2}\big)\overline{\phi}_2\right\}=0 \tag{15}$$

$$\frac{1}{i}\partial_t u_{1,2}-\mathbf{\Delta}u_{1,2}+N^{-1}v^N_{1-2}u_{1,2}+v^N_{1-2}\phi_1\phi_2=0 \tag{16}$$

Notice that $N^{-1}v^N=N^2v(N\cdot)$. If we make the change of variables (in the second equation),

$$\begin{aligned}
&x:=(x_1+x_2)/2 \quad \text{and} \quad y:=x_1-x_2 \quad \text{then we have,}\\
&\frac{1}{i}\partial_t u_{x,y}-\Delta_x u_{x,y}+\big(-2\Delta_y+N^2v(Ny)\big)u_{x,y}=-N^3v(Ny)\Phi(t,x,y)\\
&\text{where} \quad \Phi(t,x,y):=\phi(t,x+y/2)\phi(t,x-y/2)
\end{aligned}$$

One can see from the above that an "approximate" solution is $u = -Nf(Ny)\Phi(t,x,y)$ where f satisfies

$$-2\Delta f + vf = v \quad \text{or} \quad -\Delta(f-1) + \frac{1}{2}v(f-1) = 0$$

Substituting in the first equation we get

$$\frac{1}{i}\partial_t\phi_1 - \Delta\phi_1 + \int dx_2 \left\{N^3 v(N(x_1-x_2)\big(1 - f(N(x_1-x_2))\big)\overline{\phi}_2\right\}$$

and

$$\int dx \left\{v(1-f)\right\} = 8\pi a \ .$$

There is more to the coupled system. For example it describes a certain type of condensate depletion (see the conservation of particles equation). The emergence of the scattering length is due only to energy transfer.

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