ON THE SUPPORT OF COMPRESSED MODES*

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Abstract. Compressed modes are solutions of the Laplace equation with a potential and a subgradient term. The subgradient term comes from addition of an L^1 penalty in the corresponding variational principle. This paper presents an analysis of compressed modes, finding the minimizer of the variational principle, showing the spatial localization property of compressed modes, and establishing an upper bound on the volume of their support.

Key words. Compressed Modes, Sparsity, Compressive Sensing, PDE, L^1-regularization.

AMS subject classifications. 49J20, 65K10

1. Introduction.

Spatial localization occurs naturally in many problems from physics and other disciplines. A new methodology was developed in [15, 16] using sparsity techniques to obtain localized functions that are approximate solutions to a class of problems in mathematical physics that can be recast as variational optimization problems.

After introduction of an L^1 regularization term in the variational formulation of the Schrödinger equation of quantum mechanics, localized functions called "compressed modes" (CMs) were constructed by solution of the resulting new non-convex optimization problem. Numerical computation showed that the CMs have many desirable features; for example, the energy calculated using CMs approximates the ground state energy of the system (see [1, 2, 20] for proof of this statement). Moreover, there is no requirement to cut off the resulting CMs "by hand". In addition, the ideas of [15] were used in [16] to generate a new set of spatially localized orthonormal functions, called "compressed plane waves" (CPWs), with multi resolution capabilities adapted for the Laplace operator.

Several analytic treatments of CMs and CPWs have been performed. In [1] it was proven that as the L^1 regularization term vanishes in the variational formulation of the Schrödinger equation, the resulting CMs converge to a unitary transformation of the eigenfunctions of the Hamiltonian in L^2 norm. Moreover, [1] verified a conjecture in [15] that as the L^1 regularization term vanishes, the eigenvalues associated with CMs converge to the eigenvalues of the Hamiltonian. In [19, 20], CMs were proved to form a complete basis set in their corresponding vector spaces, which is necessary for use of CMs in numerical computation.

Use of the L^1 norm as a constraint or penalty term to achieve sparsity has attracted considerable attention in a variety of fields including compressed sensing [8, 9], matrix completion [17], phase retrieval [7], etc. Recently, use of sparsity techniques began in physical science (see for example [14]) and partial differential equations (see for example [18]). In all these examples sparsity means that in the representation of a corresponding vector or function in terms of a well-chosen set of modes (i.e., a basis

*The research of Caflisch and Barekat was partially supported by Department of Energy grant number DOE-SC0010613. The research of Osher was partially supported by ONR N00014-11-1-719.

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or dictionary), most coefficients are zero. However, the remarkable result of [3] and [4] proved that insertion of L^1 terms into the variational quantity for certain elliptic and parabolic PDEs would result in compact support (which can be thought as spatial sparsity) for their solutions. In [15, 16], L^1 norm regularization is used to achieve spatial sparsity for variational problems in mathematics and physics. In more recent work, [6] presents qualitative analysis of elliptic and parabolic PDEs with subgradient terms that come from L^1 regularization in the variational formulation of the problem.

The main contribution of this paper is to analytically prove the spatial localization property of CMs that was observed numerically in [15] and to show that the minimizer of the variational problem is a CM. We also prove that as the coefficient increases for the L^1 regularization term in the variational formulation of the Schrödinger equation, the volume of the support of CMs shrinks. To be specific, let $\{\psi_i\}_{i=1}^N$ denote the CMs, corresponding to number N and regularization parameter μ, that solve the L^1 regularization of the variational formulation of the Schrödinger equation in $\mathbb{R}^d$:

$$\{\psi_1,\ldots,\psi_N\} = \underset{\tilde{\psi}_1,\ldots,\tilde{\psi}_N}{\operatorname{argmin}} \sum_{i=1}^{N} \left(\frac{1}{\mu}\|\tilde{\psi}_i\|_1 + \langle \tilde{\psi}_i, \hat{H}\tilde{\psi}_i\rangle \right) \quad \text{s.t.} \quad \langle \tilde{\psi}_j, \tilde{\psi}_k\rangle = \delta_{jk}. \tag{1.1}$$

Here, $\hat{H} = -\frac{1}{2}\Delta + V(\mathbf{x})$ is the Hamiltonian operator corresponding to potential $V(\mathbf{x})$, L^1 norm is defined as $\|f\|_1 = \int_\Omega |f| d\mathbf{x}$, and $\langle f, g\rangle = \int_\Omega f^* g d\mathbf{x} \quad (\Omega \subset \mathbb{R}^d)$.

Note that the space of feasible functions in (1.1) is not a convex set, because of the orthonormality condition, and many convex optimization techniques cannot be applied here. Throughout this paper, we denote Lebesgue measure of set $A \in \mathbb{R}^d$ by $|A|$. In theorem 4.1 we show that for sufficiently small μ,

$$|\operatorname{supp}(\psi_i)| < C\mu^{2d/(4+d)} \qquad \text{for } i = 1,\ldots,N,$$

where C is a constant. This result, in particular, verifies the observations in [15] that for smaller μ, the corresponding CMs become more spatially localized.

The remainder of this paper consists of the following: Section 2 describes a set of assumptions and notations that are used in the paper. Section 3 provides an analytic formula for the first compressed mode when $V(\mathbf{x}) = 0$. Section 4 contains the main result of this paper and establishes the asymptotic upper bound on the volume of the support of compressed modes mentioned above. Section 5 includes several remarks regarding CMs corresponding to different regularization parameter μ and a conjecture. Section 6 presents some concluding remarks. Three appendices contain details: Section 7 contains the proof of the main existence theorem. Section 8 presents a proof that the first compressed mode is the unique minimizer (unique up to spatial translation) for the variational problem (as long as μ is large enough so that the compressed mode fits into the domain) and Section 9 provides a phase plane analysis of the PDE in dimension $d = 1$.

2. Assumptions and Framework. In this section we establish a set of assumptions and the framework that is used (unless the contrary is stated) throughout the paper.

Henceforth, let $\Omega = B(\mathbf{0}, L) \subset \mathbb{R}^d$ denote the d-dimensional ball of radius L centered at the origin. We impose zero boundary conditions on Ω, therefore the class of admissible functions we consider here are

$$H_0^1(\Omega) = \{w \in H_0^1(\Omega) | w = 0 \text{ on } \partial\Omega \text{ in the trace sense}\}$$

Using integration by parts in (1.1), we see that the first N compressed modes $\{\psi_i\}_{i=1}^N$ solve the following constrained optimization problem
(2.1)

$$\{\psi_1,\ldots,\psi_N\} = \underset{\tilde{\psi}_1,\ldots,\tilde{\psi}_N}{\operatorname{argmin}} \sum_{i=1}^{N} \int_\Omega (\frac{1}{\mu}|\tilde{\psi}_i| + \frac{1}{2}|\nabla\tilde{\psi}_i|^2 + V(\mathbf{x})\tilde{\psi}_i^{\,2}) d\mathbf{x} \quad \text{s.t.} \int_\Omega \tilde{\psi}_j\tilde{\psi}_k d\mathbf{x} = \delta_{jk}.$$

Throughout the paper, we assume that potential $V(\mathbf{x})$ is bounded above by a finite number; that is,

$$\|V\|_\infty := \sup_\Omega |V(\mathbf{x})| < \infty.$$

Furthermore, we assume that ψ_i's are real functions; generalization to complex-valued functions is straightforward. Also, we denote the L^p norm of a function by the standard notation:

$$\|f\|_p = \left(\int_\Omega |f|^p \,\mathrm{d}\mathbf{x}\right)^{1/p}.$$

In general, to ensure that a constrained variational problem has a minimizer, the Lagrangian (i.e., the integral operator in (1.1)) and the functions that define the constraints need to satisfy certain conditions. Typical conditions required to prove existence of minimizers are a coercivity condition and convexity of Lagrangian in terms of the differentials. It is easy to see that the Lagrangian in variational problem (2.1) satisfies these two conditions. Moreover, the functions that define the constraints in problem (2.1) are well behaved and bounded above by quadratic functions. For completeness, in appendix section 7, we provide the proof of the following theorem.

THEOREM 2.1. *There exist a minimizer to problem (2.1).*

On the other hand, we do not make any claim on the uniqueness of the solutions in variational problem (2.1). In particular, if we eliminate the L^1 term in problem (2.1) (i.e. formally set $\mu = \infty$), then any unitary transformation of solutions $\{\psi_i\}_{i=1}^N$ is also a minimizer to the variational problem. In the special case $N = 1$ and for sufficiently small values of μ, however, we will show that the minimizer has compact support and is unique, up to a spatial shift, since compact modes whose support does not touch the boundary can be shifted in space.

3. First Compressed Mode with Zero Potential. This section provides an analytic formula for the first compressed mode, for potential $V(\mathbf{x}) = 0$. This formula was formally derived in [15, equation 9], under symmetry and positivity assumptions which are proved here. The result is used later in the proof of theorem 4.1.

As before, define functional $J : H_0^1(\Omega) \to \mathbb{R}$ by

$$J[f] := \frac{1}{\mu}\|f\|_1 + \langle f, \hat{H}f\rangle = \frac{1}{\mu}\int_\Omega |f| \,\mathrm{d}\mathbf{x} + \frac{1}{2}\int_\Omega |\nabla f|^2 \,\mathrm{d}\mathbf{x} + \int_\Omega V(\mathbf{x})f(\mathbf{x})^2 \,\mathrm{d}\mathbf{x}.$$

The second equality is followed by integration by parts and using the assumptions on the boundary conditions of Ω. By the first compressed mode ψ, we mean the minimizer of $J[\psi]$ subject to the constraint that $\|\psi\|_2 = 1$.

PROPOSITION 3.1. *For $V(\mathbf{x}) = 0$, the first compressed mode ψ can be chosen to be symmetric, i.e. $\psi(\mathbf{x}) = \psi(|\mathbf{x}|)$, nonnegative and nonincreasing as a function of $|\mathbf{x}|$.*

Proof: First we show that the first compressed mode can be taken to be nonnegative. Take the function ψ, which may have positive and negative values, and replace it by $|\psi|$. Since this does not change the values of $|\psi|$ and $|\nabla\psi|$, it does not change the values of the L^2 norm or of J. It follows that $|\psi|$ is also a minimizer of J.

Let ψ^* denote the symmetric decreasing rearrangement of ψ (i.e., see for example [12]). By construction ψ^* is spherically symmetric and nonincreasing, and

$$\|\psi\|_p = \|\psi^*\|_p \qquad \text{for } 1 \leq p. \tag{3.1}$$

Moreover, Pólya-Szegő inequality says that

$$\|\nabla\psi^*\|_2 \leq \|\nabla\psi\|_2. \tag{3.2}$$

Equations (3.1) and (3.2) imply that $\|\psi^*\|_2 = 1$ and $J[\psi^*] \leq J[\psi]$. In addition, since $\psi = 0$ on $\partial\Omega$ then $\psi^* = 0$ on $\partial\Omega$; so that $\psi^* \in H_0^1(\Omega)$. It follows that ψ^* is a spherically symmetric and nonincreasing minimizer of J. This completes the proof of the proposition.

Next, we find an explicit expression for the first compressed mode when $V = 0$; that is, the minimizer of the variational problem:

$$\psi_1 = \underset{\psi}{\operatorname{argmin}} \frac{1}{\mu}\int_\Omega |\psi| d\mathbf{x} - \frac{1}{2}\int_\Omega \psi\Delta\psi d\mathbf{x} \qquad \text{s.t.} \qquad \int_\Omega \psi(\mathbf{x})^2 d\mathbf{x} = 1. \tag{3.3}$$

First consider $d = 1$ (thus $\Omega = [-L, L]$). The Euler-Lagrange equation in $1D$ is

$$-\partial_x^2\psi_1 + \frac{1}{\mu}p(\psi_1) = \lambda\psi_1 \tag{3.4}$$

in which $p(\psi)$ is the subgradient of $|\psi|$. Using the result of proposition 3.1 (i.e., that ψ_1 is spherically symmetric), the solution of (3.3) is

$$\psi_1 = \begin{cases} \dfrac{1}{\lambda\mu}[1 + \cos(\sqrt{\lambda}x)] & \text{if} \quad |x| \leq l, \\ 0 & \text{if} \quad l \leq |x| \leq L, \end{cases} \tag{3.5}$$

where $l = \pi/\sqrt{\lambda}$ and $\lambda = (3\pi)^{2/5}\mu^{-4/5}$. Here ψ_1 has compact support $[-l, l]$ if μ is small enough satisfying $l = \pi/\sqrt{\lambda} < L$. Note that $\psi_1 = \partial_x\psi_1 = 0$ and $\partial_x^2\psi_1$ has a jump of $-\mu^{-1}$ at the boundary $x = l$ of the support of ψ_1, which are all consistent with equation (3.4). From this simple 1D example, it is clear that L^1 regularization can naturally truncate solutions to the variational problem given by equation (3.3). Moreover, we also observe that the smaller μ will provide a smaller region of compact support.

The 1D solution (3.5) can be generalized to dimension $d \geq 1$, as

$$\psi_1 = \begin{cases} \dfrac{1}{\lambda\mu}(1 - U_1^{-1}U(\sqrt{\lambda}|\mathbf{x}|)) & \text{if} \quad |\mathbf{x}| \leq l, \\ 0 & \text{if} \quad l \leq |\mathbf{x}| \leq L, \end{cases} \tag{3.6}$$

in which $U = U(\rho = |\mathbf{y}|)$ (for $\mathbf{y} \in \mathbb{R}^d$) is the solution of $\Delta U = -U$, i.e.,

$$\rho^2\partial_\rho^2 U + (d-1)\rho\partial_\rho U + \rho^2 U = 0, \tag{3.7}$$

and $U_1 = U(\rho_1)$, $l = \rho_1/\sqrt{\lambda}$, $\lambda = \mu^{-4/(d+4)} I_1^{2/(d+4)}$. Here ρ_1 is the smallest (non-negative) solution of $\partial_\rho U(\rho) = 0$ and $I_1 = \int_{|\mathbf{y}|<\rho_1} (1 - U_1^{-1}U(|\mathbf{y}|))^2 \, d\mathbf{y}$ in which $\mathbf{y}$ is in $\mathbb{R}^d$. For $d = 2$, $U(\rho) = J_0(\rho)$ is the 0-th Bessel function of the first kind, and for $d = 3$, $U(\rho) = \mathrm{sinc}(\rho) = \sin(\rho)/\rho$. A proof of the following proposition is given in the appendix Section 8.

PROPOSITION 3.2. *When potential $V(\mathbf{x}) = 0$ for all $\mathbf{x} \in \Omega$ and μ is sufficiently small, then the first compressed mode ψ_1 is given by (3.6) for any dimension $d \geq 1$, and ψ_1 is the unique minimizer (unique up to spatial translation) of $J[u]$ for all admissible functions defined on Ω with $u = 0$ on $\partial\Omega$. Moreover, for $d = 1$, ψ_1 given by (3.6) is also the minimum energy solution for periodic problem as well.*

The condition on μ for Propositions 3.2 and 3.4 is that the radius L of Ω must satisfy $L \geq r_1$, and (8.14) is an explicit express for r_1.

For domains that are not symmetric or bounded, the following more general proposition is proved in the appendix Section 8:

PROPOSITION 3.3. *Let Ω be any domain in $\mathbb{R}^d$ that contains the support of the first compressed mode ψ_1 (after a spatial shift), and let potential $V(\mathbf{x}) = 0$ for all $\mathbf{x} \in \Omega$. Then ψ_1 given by (3.6) is the first compressed mode, and ψ_1 is the unique minimizer (unique up to spatial translation) of $J[u]$, among all admissible functions defined on Ω with $u = 0$ on $\partial\Omega$ and $u(x) \to 0$ as $|x| \to \infty$ in Ω.*

The following proposition follows directly from (3.6):

PROPOSITION 3.4. *When potential $V(\mathbf{x}) = 0$ for all $\mathbf{x} \in \Omega$ and μ is sufficiently small, the volume of the support of the first compressed mode ψ_1 is proportional to $\mu^{2d/(4+d)}$, where the proportionality constant depends only on d. Moreover,*

$$\int_\Omega \left(\frac{1}{\mu}|\psi_1| + \frac{1}{2}|\nabla\psi_1|^2\right) d\mathbf{x} = C_1 \mu^{-4/(4+d)},$$

where C_1 is some fixed constant depending on d.

Proof: From equation (3.6), observe that support of the first compressed mode is a sphere of radius l. Since l is proportional to $\mu^{2/(4+d)}$, the volume of the sphere is proportional to $\mu^{2d/(4+d)}$.

The second part of the proposition also follows from equation (3.6) by straightforward calculations (also see equations (8.3) and (8.5)).

4. Bounds on the Volume of Support of Compressed Modes.

This section contains the main result of the paper. In theorem 4.1, we establish an asymptotic upper bound on the volume of the support of compressed modes (CMs) in terms of regularization parameter μ. This shows that CMs are spatially localized.

THEOREM 4.1. *Using the above notation, there exist μ_0, depending on values of L, N, and d, such that for $\mu < \mu_0$ the corresponding compressed modes $\{\psi_i\}_{i=1}^N$ satisfy*

$$|supp(\psi_i)| < C\mu^{2d/(4+d)} \qquad for \qquad i = 1, \ldots, N.$$

Here, C is a constant whose value depends on N, d, and $\|V\|_\infty$.

Proof: The proof consists of four parts:

Step 1: Finding Euler-Lagrange equations

For any function u, let $p(u)$ denote an element of subdifferential of $|u|$, that is

$$p(u) = \begin{cases} 1 & \text{if } u > 0 \\ \in [-1, 1] & \text{if } u = 0 \\ -1 & \text{if } u < 0. \end{cases}$$

From the theory of variational calculus with constraints (i.e., see for example [10, Chapter 8]) we know that the solutions of (2.1) are weak solutions of the following system of nonlinear boundary value problem:

For $i = 1, \dots, N$,

$$\frac{1}{\mu}p(\psi_i) + (2V(\mathbf{x}) - 2\lambda_i)\psi_i - \Delta\psi_i - \sum_{j\neq i}\lambda_{ij}\psi_j = 0 \qquad \text{in } \Omega \tag{4.1}$$

where constants λ_i and λ_{ij} (with $\lambda_{ij} = \lambda_{ji}$) are Lagrange multipliers corresponding to orthonormality constraints

$$\int_\Omega \psi_i^2 d\mathbf{x} = 1, \qquad \text{and} \qquad \int_\Omega \psi_i\psi_j d\mathbf{x} = 0, \qquad \text{for } i, j = 1, \dots, N. \tag{4.2}$$

Satisfying the Euler-Lagrange equations (4.1) is a necessary but not sufficient condition for solutions of (2.1).

Step 2: Upper bounds for λ_i, $\|\psi_i\|_1$, and $\|\nabla\psi_i\|_2$

For each i multiply both sides of equation (4.1) by $\psi_i(\mathbf{x})$ and integrate over domain Ω:

$$\int_\Omega \left(\frac{1}{\mu}p(\psi_i)\psi_i + (2V(\mathbf{x}) - 2\lambda_i)\psi_i^2 - (\Delta\psi_i)\psi_i - \sum_{j\neq i}\lambda_{ij}\psi_j\psi_i\right) d\mathbf{x} = 0,$$

which, using orthonormality conditions (4.2) and integration by parts, implies that

$$\frac{1}{\mu}\int_\Omega |\psi_i| d\mathbf{x} + 2\int_\Omega V(\mathbf{x})\psi_i^2 d\mathbf{x} - 2\lambda_i + \int_\Omega |\nabla\psi_i|^2 d\mathbf{x} = 0.$$

Therefore,

$$\lambda_i = \frac{1}{2\mu}\int_\Omega |\psi_i| d\mathbf{x} + \int_\Omega V(\mathbf{x})\psi_i^2 d\mathbf{x} + \frac{1}{2}\int_\Omega |\nabla\psi_i|^2 d\mathbf{x}. \tag{4.3}$$

Next, let $\{f_i\}_{i=1}^N$ be the compressed modes when potential $V(\mathbf{x})$ is zero everywhere; that is:

$$\{f_1, \dots, f_N\} = \underset{\tilde{f}_1,\dots,\tilde{f}_N}{\operatorname{argmin}} \sum_{i=1}^N \int_\Omega (\frac{1}{\mu}|\tilde{f}_i| + \frac{1}{2}|\nabla\tilde{f}_i|^2) d\mathbf{x} \quad \text{s.t.} \quad \int_\Omega \tilde{f}_j\tilde{f}_k d\mathbf{x} = \delta_{jk}. \tag{4.4}$$

Observe that

$$\begin{aligned}
\sum_{i=1}^N \int_\Omega (\frac{1}{\mu}|\psi_i| + \frac{1}{2}|\nabla\psi_i|^2) d\mathbf{x} - N\|V\|_\infty &\leq \sum_{i=1}^N \int_\Omega (\frac{1}{\mu}|\psi_i| + \frac{1}{2}|\nabla\psi_i|^2 + V(\mathbf{x})\psi_i^2) d\mathbf{x} \\
&\leq \sum_{i=1}^N \int_\Omega (\frac{1}{\mu}|f_i| + \frac{1}{2}|\nabla f_i|^2 + V(\mathbf{x})f_i^2) d\mathbf{x} \\
&\leq \sum_{i=1}^N \int_\Omega (\frac{1}{\mu}|f_i| + \frac{1}{2}|\nabla f_i|^2) d\mathbf{x} + N\|V\|_\infty, \qquad (4.5)
\end{aligned}$$

where we used definition (2.1) in the second line. For the first and third line, we used orthonormality of f_j's and ψ_j's to conclude that for each j

$$
\begin{aligned}
|\int_\Omega V(\mathbf{x})\psi_j^2|d\mathbf{x} &\le \int_\Omega |V(\mathbf{x})|\psi_j^2 d\mathbf{x} \\
&\le \|V\|_\infty \\
|\int_\Omega V(\mathbf{x})f_j^2|d\mathbf{x} &\le \int_\Omega |V(\mathbf{x})|f_j^2 d\mathbf{x} \\
&\le \|V\|_\infty.
\end{aligned} \tag{4.6}
$$

Now from proposition 3.4, we know that when potential $V(\mathbf{x})$ is zero everywhere, the first compressed mode f has support whose volume is proportional to $\mu^{2d/(4+d)}$. It follows that for μ sufficiently small, N disjoint copies (i.e. translates) of f can be placed in Ω, and these N functions are a solution for problem (4.4). Therefore, in view of proposition 3.4, there exist μ_0 (depending on values of L, N and d) such that for $\mu < \mu_0$:

$$
\sum_{i=1}^N \int_\Omega (\frac{1}{\mu}|f_i| + \frac{1}{2}|\nabla f_i|^2) d\mathbf{x} = C_1 N \mu^{-4/(4+d)},
$$

for some fixed constant C_1, depending on d. Using this in equation (4.5) and rearranging, we have

$$
\sum_{i=1}^N \int_\Omega \frac{1}{\mu}|\psi_i| d\mathbf{x} + \sum_{i=1}^N \int_\Omega \frac{1}{2}|\nabla \psi_i|^2 d\mathbf{x} \le C_1 N \mu^{-4/(4+d)} + 2N\|V\|_\infty.
$$

Because each of the summands in the left hand side of above inequality is positive, there exist constant C_2 (i.e., depending on d, N and $\|V\|_\infty$) such that for $\mu < \mu_0$,

$$
\int_\Omega \frac{1}{\mu}|\psi_i| d\mathbf{x} < C_2 \mu^{-4/(4+d)} \quad \text{and} \quad \int_\Omega |\nabla \psi_i|^2 d\mathbf{x} < C_2 \mu^{-4/(4+d)} \quad \text{for} \quad i = 1, \dots, N. \tag{4.7}
$$

Moreover, substituting the above inequalities into (4.3) and using (4.6), it follows that there exist constant C_3 (depending on d, N and $\|V\|_\infty$) such that for $\mu < \mu_0$

$$
|\lambda_i| < \frac{C_2}{2}\mu^{-4/(4+d)} + \|V\|_\infty + \frac{C_2}{2}\mu^{-4/(4+d)} < C_3 \mu^{-4/(4+d)}. \tag{4.8}
$$

Step 3: Upper bounds for λ_{ij}'s

Fix i. For $k \neq i$ multiply both sides of equation (4.1) by $\psi_k(\mathbf{x})$ and integrate over Ω:

$$
\int_\Omega \left(\frac{1}{\mu} p(\psi_i)\psi_k + (2V(\mathbf{x}) - 2\lambda_i)\psi_i\psi_k - (\Delta\psi_i)\psi_k - \sum_{j\neq i} \lambda_{ij}\psi_j\psi_k \right) d\mathbf{x} = 0,
$$

which, using orthonormality conditions (4.2) and integration by parts, implies that

$$
\frac{1}{\mu}\int_\Omega p(\psi_i)\psi_k d\mathbf{x} + 2\int_\Omega V(\mathbf{x})\psi_i\psi_k d\mathbf{x} + \int_\Omega (\nabla\psi_i)\cdot(\nabla\psi_k) d\mathbf{x} - \lambda_{ik} = 0.
$$

Therefore,

$$\lambda_{ik} = \frac{1}{\mu}\int_\Omega p(\psi_i)\psi_k d\mathbf{x} + 2\int_\Omega V(\mathbf{x})\psi_i\psi_k d\mathbf{x} + \int_\Omega (\nabla\psi_i)\cdot(\nabla\psi_k)d\mathbf{x}. \tag{4.9}$$

In view of (4.7),

$$\left|\frac{1}{\mu}\int_\Omega p(\psi_i)\psi_k d\mathbf{x}\right| \le \frac{1}{\mu}\int_\Omega |\psi_k| d\mathbf{x} < C_2\mu^{-4/(4+d)}.$$

Also, note that by Cauchy-Schwarz and orthonormality of ψ_i and ψ_k,

$$\begin{aligned}\left|\int_\Omega V(\mathbf{x})\psi_i\psi_k d\mathbf{x}\right| &\le \|V\|_\infty \int_\Omega |\psi_i||\psi_k| d\mathbf{x}\\ &\le \|V\|_\infty \left(\int_\Omega \psi_i^2 d\mathbf{x}\right)^{1/2}\left(\int_\Omega \psi_k^2 d\mathbf{x}\right)^{1/2}\\ &= \|V\|_\infty.\end{aligned}$$

Finally, using Cauchy-Schwarz and equation (4.7),

$$\begin{aligned}\int_\Omega (\nabla\psi_i)\cdot(\nabla\psi_k)d\mathbf{x} &\le \left(\int_\Omega |\nabla\psi_i|^2 d\mathbf{x}\right)^{1/2}\left(\int_\Omega |\nabla\psi_k|^2 d\mathbf{x}\right)^{1/2}\\ &< (C_2\mu^{-4/(4+d)})^{1/2}(C_2\mu^{-4/(4+d)})^{1/2} = C_2\mu^{-4/(4+d)}.\end{aligned}$$

Substituting, the last three inequalities into equation (4.9), shows that for $\mu < \mu_0$

$$|\lambda_{ik}| < C_2\mu^{-4/(4+d)} + 2\|V\|_\infty + C_2\mu^{-4/(4+d)} < C_4\mu^{-4/(4+d)}, \tag{4.10}$$

where constant C_4 depends on d, N, and $\|V\|_\infty$.

Step 4: Bounding the volume of the support of ψ_i's

For each i multiply both sides of equation (4.1) by

$$\operatorname{sgn}(\psi_i) = \begin{cases} 1 & \text{if } \psi_i > 0\\ 0 & \text{if } \psi_i = 0\\ -1 & \text{if } \psi_i < 0\end{cases}$$

and integrate over domain Ω. It follows that

$$\frac{1}{\mu}|\operatorname{supp}(\psi_i)| + \int_\Omega (2V(\mathbf{x}) - 2\lambda_i)|\psi_i| d\mathbf{x} - \int_\Omega \operatorname{sgn}(\psi_i)\Delta\psi_i d\mathbf{x} - \sum_{j\neq i}\lambda_{ij}\int_\Omega \psi_j \operatorname{sgn}(\psi_i) d\mathbf{x} = 0. \tag{4.11}$$

Define

$$\Omega^+ = \{\mathbf{x}\in\Omega : \psi_i(\mathbf{x}) > 0\},$$

and

$$\Omega^- = \{\mathbf{x}\in\Omega : \psi_i(\mathbf{x}) < 0\}.$$

According to Green's formula

$$\int_{\Omega^+} \Delta\psi_i d\mathbf{x} = \int_{\partial\Omega^+} \frac{\partial\psi_i}{\partial\nu} dS \le 0,$$

where ν is outward pointing unit normal vector along $\partial\Omega^+$. Since ψ_i is positive in Ω^+ and becomes zero on $\partial\Omega^+$ (i.e. note that since ψ_i is a solution to the Euler–Lagrange equation (4.1), it is continuous), the RHS of above expression is not positive. In order to apply Green's theorem, we need $\partial\Omega^+$ to be continuously differentiable. Nevertheless, if this is not the case, we approximate function ψ_i by a sequence of functions for which the corresponding boundary is C^1, and we can still conclude the above inequality.

With a similar argument, we have that

$$\int_{\Omega^-} \Delta\psi_i d\mathbf{x} \geq 0.$$

Hence,

$$\int_{\Omega} \operatorname{sgn}(\psi)\Delta\psi_i d\mathbf{x} = \int_{\Omega^+} \Delta\psi_i d\mathbf{x} - \int_{\Omega^-} \Delta\psi_i d\mathbf{x} \leq 0. \tag{4.12}$$

Using inequality (4.12) in (4.11) and rearranging, we conclude that

$$\begin{aligned}
&\frac{1}{\mu}|\operatorname{supp}(\psi_i)| \\
&\leq \int_{\Omega} |2\lambda_i - 2V(\mathbf{x})|\; |\psi_i| d\mathbf{x} + \sum_{j\neq i} \lambda_{ij} \int_{\Omega} |\psi_j| d\mathbf{x} \\
&\leq (2\lambda_i + 2\|V\|_\infty) \int_{\Omega} |\psi_i| d\mathbf{x} + \sum_{j\neq i} \lambda_{ij} \int_{\Omega} |\psi_j| d\mathbf{x} \\
&\leq (2C_3\mu^{-4/(4+d)} + 2\|V\|_\infty)(\mu C_2\mu^{-4/(4+d)}) + (N-1)C_4\mu^{-4/(4+d)}(\mu C_2\mu^{-4/(4+d)}),
\end{aligned}$$

where the last line comes from equations (4.8), (4.10) and (4.7). Hence, there exist constant C depending on N, d, and $\|V\|_\infty$ such that, for each $i = 1, \ldots, N$, when $\mu < \mu_0$ (recall that μ_0 depends on L, N and d)

$$|\operatorname{supp}(\psi_i)| \leq C\mu^{2d/(4+d)}.$$

This completes the proof of theorem 4.1.

Remark 4.2. *In view of proposition 3.4, the asymptotic bound of theorem 4.1 is tight for the case $V(\mathbf{x}) = 0$.*

Remark 4.3. *Note that the upper bound estimate for the volume of the support of compressed modes is independent of the value of L. The value of L becomes important only in determining the value of μ_0. Indeed, as $L \to \infty$, $\mu_0 \to \infty$.*

5. Effect of Regularization Term. As noted earlier, the regularization parameter μ controls how spatial localization of the corresponding compressed modes are. Indeed, in section 4 we demonstrated that the volume of the support of compressed modes is bounded above by a quantity that depends on μ. It is of interest to establish relationships between different sets of compressed modes corresponding to different values of regularization parameter μ. To be specific, let $\{\psi_i^{(1)}\}_{i=1}^N$ and $\{\psi_i^{(2)}\}_{i=1}^N$ be the CMs corresponding to parameters μ_1 and μ_2, with $\mu_1 < \mu_2$. That is,

$$\{\psi_1^{(1)}, \ldots, \psi_N^{(1)}\} = \operatorname*{argmin}_{\tilde\psi_1,\ldots,\tilde\psi_N} \sum_{i=1}^N \frac{1}{\mu_1}\|\tilde\psi_i\|_1 + \langle\tilde\psi_i, \hat H\tilde\psi_i\rangle \quad \text{s.t.} \quad \langle\tilde\psi_j, \tilde\psi_k\rangle = \delta_{jk}, \tag{5.1}$$

and

$$\{\psi_1^{(2)}, \ldots, \psi_N^{(2)}\} = \underset{\tilde{\psi}_1,\ldots,\tilde{\psi}_N}{\operatorname{argmin}} \sum_{i=1}^{N} \frac{1}{\mu_2}\|\tilde{\psi}_i\|_1 + \langle \tilde{\psi}_i, \hat{H}\tilde{\psi}_i\rangle \quad \text{s.t.} \quad \langle \tilde{\psi}_j, \tilde{\psi}_k\rangle = \delta_{jk}. \tag{5.2}$$

PROPOSITION 5.1. *Using the above notation,*

$$\sum_{i=1}^{N} \|\psi_i^{(1)}\|_1 \leq \sum_{i=1}^{N} \|\psi_i^{(2)}\|_1.$$

Proof: By way of contradiction, assume that

$$\sum_{i=1}^{N} \|\psi_i^{(2)}\|_1 < \sum_{i=1}^{N} \|\psi_i^{(1)}\|_1.$$

Multiplying both sides by $(1/\mu_1 - 1/\mu_2) > 0$, gives

$$\sum_{i=1}^{N}(\frac{1}{\mu_1} - \frac{1}{\mu_2})\|\psi_i^{(2)}\|_1 < \sum_{i=1}^{N}(\frac{1}{\mu_1} - \frac{1}{\mu_2})\|\psi_i^{(1)}\|_1. \tag{5.3}$$

On the other hand, minimality property of (5.2) implies

$$\sum_{i=1}^{N} \frac{1}{\mu_2}\|\psi_i^{(2)}\|_1 + \langle \psi_i^{(2)}, \hat{H}\psi_i^{(2)}\rangle \leq \sum_{i=1}^{N} \frac{1}{\mu_2}\|\psi_i^{(1)}\|_1 + \langle \psi_i^{(1)}, \hat{H}\psi_i^{(1)}\rangle. \tag{5.4}$$

Adding both sides of equations (5.3) and (5.4), yields

$$\sum_{i=1}^{N} \frac{1}{\mu_1}\|\psi_i^{(2)}\|_1 + \langle \psi_i^{(2)}, \hat{H}\psi_i^{(2)}\rangle \leq \sum_{i=1}^{N} \frac{1}{\mu_1}\|\psi_i^{(1)}\|_1 + \langle \psi_i^{(1)}, \hat{H}\psi_i^{(1)}\rangle.$$

This last equation, contradicts the minimality property of (5.1). The result follows.

The above proposition shows that as μ decreases, the sum of the L^1-norm of the corresponding compressed modes decreases monotonically. We conjecture that the sum of the volume of the support of compressed modes also decreases monotonically as μ decreases:

CONJECTURE 5.2. *Using the above notation,*

$$\sum_{i=1}^{N} |supp(\psi_i^{(1)})| \leq \sum_{i=1}^{N} |supp(\psi_i^{(2)})|.$$

6. Conclusion. In this paper we establish an asymptotic upper bound on the volume of the support of compressed modes, which were introduced in [15] as a way of finding spatially localized approximate solutions for the Schrödinger operator. This proves that compressed modes are spatially localized.

The result of this paper can also be used to find an a prior estimate on the value of regularization parameter μ required in the variational problem, in order to achieve a desired level of localization in the compressed modes.

Acknowledgments. F. B. is thankful of Marek Biskup for helpful conversations. The authors are thankful of the anonymous referees for their insightful remarks and helpful comments.

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7. Existence of Minimizer. In this appendix, we prove Theorem 2.1.

For ease of exposition the result is shown for the case of $N = 1$. The proof readily extends to general N with the only new complications being notational. The proof outlined here generally mimics the arguments provided in Theorem 1 in section 8.4.1 and Theorem 2 in section 8.2.2 of [10].

Define energy functional $J : H_0^1(\Omega) \to \mathbb{R}$ by

$$J[f] := \int_\Omega \frac{1}{\mu}|f| + \frac{1}{2}|\nabla f|^2 + V(\mathbf{x})f(\mathbf{x})^2 \ \mathrm{d}\mathbf{x},$$

and constrained functional by

$$I[f] := \int_{\Omega} |f|^2 \, \mathrm{d}\mathbf{x}.$$

Therefore, the feasible class of functions for the minimization problem is

$$\mathcal{A} = \{f \in H_0^1(\Omega) \mid I[f] = 1\}.$$

The goal is to show that there exist $\psi \in \mathcal{A}$ satisfying

$$J[\psi] = \min_{f \in \mathcal{A}} J[f].$$

The rest of the proof consists of three steps:

Step1: Set $m = \inf_{f\in\mathcal{A}} J[f]$. Because Ω is bounded, it is clear that m is finite (indeed, note that a simple application of Cauchy-Schwarz shows that m is bounded below by $-\|V\|_\infty$). Choose a minimizing sequence $\{f_k\}_{k=1}^\infty \subset \mathcal{A}$ with

$$J[f_k] \to m. \tag{7.1}$$

Step 2: Now it is shown that $\{f_k\}_{k=1}^\infty$ has a weakly convergent subsequence in $H_0^1(\Omega)$. Note that if $f \in \mathcal{A}$ then

$$\begin{aligned} J[f] &= \int \frac{1}{\mu}|f| + \frac{1}{2}|\nabla f|^2 + V(\mathbf{x})f(\mathbf{x})^2 \, \mathrm{d}\mathbf{x} \\ &\geq \frac{1}{\mu}\int |f| \, \mathrm{d}\mathbf{x} + \int \frac{1}{2}|\nabla f|^2 \, \mathrm{d}\mathbf{x} - \|V\|_\infty \int |f(x)|^2 \, \mathrm{d}\mathbf{x} \\ &\geq 0 + \frac{1}{2}\|\nabla f\|_2^2 - \|V\|_\infty \|f\|_2^2 \\ &= \frac{1}{2}\|\nabla f\|_2^2 - \|V\|_\infty. \end{aligned}$$

In view of (7.1),

$$\sup_k \|\nabla f_k\|_2 < \infty. \tag{7.2}$$

By the Poincare's inequality, equation (7.2) implies that

$$\sup_k \|f_k\|_2 < \infty. \tag{7.3}$$

Equations (7.2) and (7.3) imply that $\{f_k\}_{k=1}^\infty$ is bounded in $H_0^1(\Omega)$. Consequently, there exist a subsequence $\{f_{k_j}\}_{j=1}^\infty \subset \{f_k\}_{k=1}^\infty$ and a function $\psi \in H_0^1(\Omega)$ such that

$$f_{k_j} \rightharpoonup \psi \quad \text{weakly in } H_0^1(\Omega). \tag{7.4}$$

Step 3: Finally, it is verified that $I[\psi] = 1$ (i.e. $\psi \in \mathcal{A}$) and $J[\psi] = m$; which completes the proof. Since $H_0^1(\Omega)$ is compactly contained in $L^2(\Omega)$, it is standard to deduce from (7.4) that

$$f_{k_j} \to \psi \quad \text{in } L^2(\Omega). \tag{7.5}$$

Now,

$$\begin{aligned}
|I[\psi]-1| &= |I[\psi]-I[f_{k_j}]| \\
&\le \int |\psi^2 - f_{k_j}^2| \ \mathrm{d}\mathbf{x} \\
&= \int |\psi - f_{k_j}|\ |\psi + f_{k_j}| \ \mathrm{d}\mathbf{x} \\
&\le \|\psi - f_{k_j}\|_2 \int |\psi + f_{k_j}|^2 \ \mathrm{d}\mathbf{x} \qquad \text{(by Cauchy-Schwarz)} \\
&\to 0 \quad \text{as } j \to \infty \text{ by (7.5)}.
\end{aligned}$$

On the other hand, let $L(\nabla f(x), f(x), x) = \frac{1}{2}|\nabla f(x)|^2 + V(x)f(x)^2$. By theorem 1 in section 8.2.2 of [10], $\int_\Omega L(\nabla f(x), f(x), x)\ \mathrm{d}\mathbf{x}$ is weakly lower semicontinuous, thus

$$\int \frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})\psi(\mathbf{x})^2 \ \mathrm{d}\mathbf{x} \le \liminf_j \left(\int \frac{1}{2}|\nabla f_{k_j}|^2 + V(\mathbf{x}) f_{k_j}(\mathbf{x})^2 \ \mathrm{d}\mathbf{x} \right).$$

Moreover, because Ω is bounded, (7.5) implies that $f_{k_j} \to \psi$ in $L^1(\Omega)$. In particular,

$$\int |\psi| \ \mathrm{d}\mathbf{x} = \lim_j \int |f_{k_j}| \ \mathrm{d}\mathbf{x}.$$

Hence, $J[\psi] \le \liminf_j J[f_{k_j}] = m$. Since by definition of m, $m \le J[\psi]$, it must be the case that $J[\psi] = m$.

This completes proof of theorem 2.1.

8. Energy Minimization. In this appendix, we prove Propositions 3.2 and 3.3. In this appendix, $V = 0$.

8.1. Proof of Proposition 3.2. Theorem 2.1 and Proposition 3.1 show that there is a minimum energy solution ψ and that it is nonnegative, non-increasing and spherically symmetric. We sometimes write $\psi(r)$ in place of $\psi(\mathbf{x})$, where $r = |\mathbf{x}|$. Let

$$r_* = \min_{\psi(r)=0} r.$$

Note that $r_* \le L$ because $\Omega = B(\mathbf{0}, L)$. The minimizer ψ satisfies the Euler-Lagrange equation

$$-\Delta\psi + \frac{1}{\mu} p(\psi) = \lambda\psi, \tag{8.1}$$

in which $p(\psi)$ is the subgradient of $|\psi|$, and $\psi = 0$ on $\partial\Omega$. Note that $\lambda \ge 0$, since otherwise (8.1) with the Dirichlet boundary condition $\psi = 0$ has no nontrivial solution. It follows that

$$\psi = \begin{cases} \frac{1}{\lambda\mu}(1 + cU(\sqrt{\lambda} r)) & \text{if} \quad |\mathbf{x}| = r \le r_*, \\ 0 & \text{if} \quad |\mathbf{x}| = r \ge r_*, \end{cases}$$

in which U solves (3.7) and c is a constant chosen to be positive. The conditions on ψ implies that $U(0) > 0$ and that U must be symmetric and non-increasing for $r \le r_*$.

Since the ODE (3.7) is linear and second order, it has two independent solutions. For $d = 1$, the only symmetric solution (up to a constant factor) is $U(r) = \cos r$; while for $d > 1$, there is only a single solution (up to a constant factor) that is nonsingular at $r = 0$. We denote ρ_0 to be the first zero of U and ρ_1 to be the first local minimum of U, which is a strict local minimum. Since $(\rho^{d-1}U'(\rho))' + \rho^{d-1}U(\rho) = 0$, one can easily show that $\rho_0 < \rho_1$, that $U(\rho) > 0$ for $0 \le \rho < \rho_0$, that $U(\rho) < 0$ for $\rho_0 < \rho < \rho_1$, and that $U'(\rho) < 0$ for $0 < \rho < \rho_1$. We also denote $(r, r_0, r_1, r_*) = \lambda^{-1/2}(\rho, \rho_0, \rho_1, \rho_*)$. The L^2 constraint on ψ (see equation 8.3 below) implies that λ is a function of ρ_*; however, to ease the notation we avoid showing the dependency explicitly.

In order for the solution $\psi(r)$ to have a zero at $r = r_*$, it must have the form

$$\psi(r) = \frac{1}{\lambda\mu}\left(1 - \frac{U(\rho)}{U(\rho_*)}\right) \tag{8.2}$$

It is easy to see that the only values of r_* for which ψ is nonnegative and nonincreasing in r are those satisfying $r_0 < r_* \le r_1$. In 1D these solutions are described through the phase plane analysis in Section 9 as the separatrices (the compactly supported solutions) and the positive part of the outer periodic solutions.

The solution with $r_* = r_1$ (i.e., the solution described in (3.5) and (3.6)) is special, since $\psi = \partial_r\psi = 0$ at $r = r_1$ (which follows from $U = U' = 0$ at $\rho = \rho_1$). Therefore this solution can be continued as $\psi = 0$ for all $r \ge r_1$; i.e., these solutions are valid for any $L \ge r_* = r_1$.

Solutions ψ with $r_0 < r_* < r_1$ have $\partial_r\psi(r_*) < 0$ and cannot be continued for $r > r_*$ (with continuous first derivative), since ψ would not be nonnegative for $r > r_*$. So these solutions are only valid for $L = r_*$.

In general the L^2 norm $I[\psi]$ is given by

$$\begin{aligned} I &= \int_{|\mathbf{x}|\le r_*} \psi^2(\mathbf{x})d\mathbf{x} \\ &= c_d \int_0^{r_*} \left\{\mu^{-1}\lambda^{-1}\left(1 - \frac{U(\sqrt{\lambda}r)}{U(\sqrt{\lambda}r_*)}\right)\right\}^2 r^{d-1}dr \\ &= c_d\mu^{-2}\lambda^{-(4+d)/2}N(\rho_*) \qquad (8.3) \end{aligned}$$

$$N(\rho_*) = \int_0^{\rho_*}\left(1 - \frac{U(\rho)}{U(\rho_*)}\right)^2 \rho^{d-1}d\rho. \tag{8.4}$$

Similarly, using integration by parts, the Euler-Lagrange equation (8.1), and the scaling as above, the energy $J[\psi]$ is given by

$$\begin{aligned} J &= \int_{|\mathbf{x}|\le r_*} \frac{1}{2}|\nabla\psi|^2 + \mu^{-1}|\psi|d\mathbf{x} \\ &= \frac{1}{2}\int_{|\mathbf{x}|\le r_*} \mu^{-1}|\psi| + \lambda\psi^2 d\mathbf{x} \\ &= \frac{1}{2}c_d\mu^{-2}\lambda^{-(2+d)/2}\left(K(\rho_*) + N(\rho_*)\right) \qquad (8.5) \end{aligned}$$

$$K(\rho_*) = \int_0^{\rho_*}\left(1 - \frac{U(\rho)}{U(\rho_*)}\right)\rho^{d-1}d\rho. \tag{8.6}$$

Note that the absolute values are omitted from K, since the integrand is positive in this interval. Also note that the formula for J will only be used for the periodic case in $d = 1$.

From (8.3) and (8.4), it is clear that $N(\rho_*) > 0$. Next we show that $N'(\rho_*) < 0$ for $\rho_0 < \rho_* < \rho_1$. A direct calculation shows that

$$\begin{aligned} N'(\rho_*) &= \int_0^{\rho_*} 2\frac{U'(\rho_*)U(\rho)}{U(\rho_*)^2}\left(1 - \frac{U(\rho)}{U(\rho_*)}\right)\rho^{d-1}d\rho \\ &= N_1' + N_2' \end{aligned} \tag{8.7}$$

in which

$$\begin{aligned} N_1' &= 2\frac{U'(\rho_*)}{U(\rho_*)^2}\int_0^{\rho_*} U(\rho)\rho^{d-1}d\rho \\ &= -2\frac{U'(\rho_*)}{U(\rho_*)^2}\int_0^{\rho_*} (U'(\rho)\rho^{d-1})'d\rho \\ &= -2\frac{U'(\rho_*)}{U(\rho_*)^2}U'(\rho_*)\rho_*^{d-1} \\ &< 0 \end{aligned} \tag{8.8}$$

$$N_2' = -2\frac{U'(\rho_*)}{U(\rho_*)^3}\int_0^{\rho_*} U(\rho)^2\rho^{d-1}d\rho \tag{8.9}$$

in which the next to last line in (8.8) comes from rewriting (3.7) as $(\rho^{d-1}U'(\rho))' + \rho^{d-1}U(\rho) = 0$. Also, since $\rho_0 < \rho_* < \rho_1$, then $U(\rho_*) < 0$ and $U'(\rho_*) < 0$, so that $N_2' < 0$. Together this shows that $N'(\rho_*) < 0$ for $\rho_0 < \rho_* < \rho_1$.

Next apply the constraint $I = 1$, so that (from (8.3)) for every value of λ there is a corresponding value of ρ_* and of $r_* = \lambda^{-1/2}\rho_*$. We denote these values as $\rho_*(\lambda)$ and $r_*(\lambda)$, and their derivatives as $\rho_*'(\lambda)$ and $r_*'(\lambda)$. With some abuse of notation, we also denote $r_*(\rho_*)$ and and its derivative as $r_*'(\rho_*) = r_*'(\lambda)/\rho_*'(\lambda)$. From (8.3), the constraint $I = 1$ implies

$$\begin{aligned} 0 &= I'(\lambda) \\ &= -\frac{4+d}{2}\lambda^{-1}I(\lambda) + \frac{N'(\rho_*)}{N(\rho_*)}I(\lambda)\rho_*'(\lambda) \end{aligned} \tag{8.10}$$

so that

$$\rho_*'(\lambda) = \frac{4+d}{2}\frac{N(\rho_*)}{\lambda N'(\rho_*)} < 0. \tag{8.11}$$

Then since $r_* = \lambda^{-1/2}\rho_*$,

$$r_*'(\lambda) = \lambda^{-1/2}\left(\rho_*'(\lambda) - \frac{1}{2}\lambda^{-1}\rho_*\right) < 0. \tag{8.12}$$

It follows that

$$r_*'(\rho_*) = \frac{r_*'(\lambda)}{\rho_*'(\lambda)} > 0. \tag{8.13}$$

Since $r_* = r_1$ for $\rho_* = \rho_1$, then $r_* < r_1$ for $\rho_0 < \rho_* < \rho_1$. It follows that for $L > r_1$, there are no solutions of the form (8.2) with $r_* < r_1$.

Uniqueness of the energy minimizer follows from the following general result [5, 11]: If $\{r : |\operatorname{grad}\psi^*(r)| = 0\} \cap \{r : 0 < \psi^*(r) < \sup\psi\} = \emptyset$, then $\int |\operatorname{grad}\psi^*|d\mathbf{x} <$

$\int |\operatorname{grad}\psi| d\mathbf{x}$ and therefore $J[\psi^*] < J[\psi]$, unless $\psi = \psi^*$ after a possible spatial translation. Since $\partial_\rho U < 0$ for $0 < \rho < \rho_1$, then $\partial_r \psi_1 < 0$ for $0 < r < r_1$, and ψ_1 has its maximum at $r = 0$ and is 0 at $r = r_1$. Moreover ψ_1 is the unique minimizer that is spherically symmetric, nonincreasing and nonnegative. It follows that ψ_1 is the unique minimizer (unique up to a spatial translation) among all admissible functions.

In summary for $L \geq r_1$, the first mode must be the function (8.2) with $r_* = r_1$. From (8.3), the value of r_1 is given by

$$\begin{aligned} r_1 &= \rho_1 \lambda^{-1/2} \\ &= \rho_1 (c_d N(\rho_1))^{-1/(4+d)} \mu^{2/(4+d)} \end{aligned} \tag{8.14}$$

in which N is given by (8.4) and ρ_1 is the first local minimum of U, with U being the nonincreasing, nonsingular solution of (3.7). The restriction $L \geq r_1$ is just the requirement that the domain is large enough to include the compressed mode.

For $d = 1$, the periodic case is somewhat different. The only solutions $\psi(x)$ that are symmetric, non-negative and non-increasing are $\psi(x) = \mu^{-1}\lambda^{-1}\left(1 - \epsilon^2 \cos(\sqrt{\lambda} x)\right)$ for $|x| < \pi/\sqrt{\lambda}$, with $0 \leq \epsilon \leq 1$. These solutions are described through the phase plane analysis in Section 8 as the periodic solutions inside the separatrices.

The amplitude and energy integrals are

$$\begin{aligned} I &= \int_{|x|<\pi\sqrt{\lambda}} \psi^2(x) dx \\ &= (2+\epsilon^2)\pi\mu^{-2}\lambda^{-5/2} \end{aligned} \tag{8.15}$$

$$\begin{aligned} J &= \int_{|x|<\pi\sqrt{\lambda}} \left(\frac{1}{2}u_x^2 + \mu^{-1}|u|\right) dx \\ &= \frac{1}{2}\int_{|x|<\pi\sqrt{\lambda}} \left(\mu^{-1}|u| + \lambda u^2\right) dx \\ &= \left(\frac{1}{2}(2+\epsilon^2)^{2/5} + (2+\epsilon^2)^{-3/5}\right) \pi^{2/5} I^{3/5} \mu^{-4/5}. \end{aligned} \tag{8.16}$$

The first term in parentheses has a minimum at $\epsilon = 1$. It follows that for $I = 1$, $J(\epsilon) \geq J(1)$ for $0 < \epsilon \leq 1$. This minimum corresponds to the solution (8.2) with $r_* = r_1$.

8.2. Proof of Proposition 3.3. Consider any admissible function u for J on Ω with $\|u\|_2 = 1$. Since u can be replaced by $|u|$ and extended as $u(\mathbf{x}) = 0$ for $\mathbf{x} \in \Omega^c$, without changing $J[u]$ or $\|u\|_2$, we can assume that u is defined on $\mathbb{R}^d$ and that $u \geq 0$. Next define u^* to be the symmetric decreasing rearrangement of u, which satisfies $J[u^*] \leq J[u]$ and $\|u^*\|_2 = 1$. If the support of u^* is bounded, then Proposition 3.2 shows that $J[\psi_1] \leq J[u^*]$, so that $J[\psi_1] \leq J[u]$. Note that this does not require that the support of u^* is contained in Ω.

If the support of u^* is unbounded, then we make a scaled cutoff of u^*, as follows: For any small positive number ε, let R be large enough that the following two inequalities are satisfied:

$$\int_{R<|\mathbf{x}|} |\nabla u^*|^2 + \mu^{-1}|u^*| + |u^*|^2 d\mathbf{x} < \varepsilon \tag{8.17}$$

$$u^*(\mathbf{x}) < \varepsilon \|u^*\|_1^{-1} \quad \text{for } |\mathbf{x}| > R. \tag{8.18}$$

Set $\bar{u} = u(2R)$, which also satisfies $\bar{u} < \varepsilon \|u^*\|_1^{-1}$, and define $u_R^* = (u^* - \bar{u})^+$, which is also symmetric and nonincreasing, with u_R^* for $|\mathbf{x}| > 2R$. Since u^* is decreasing, then $\bar{u} < u^*$ for $R < |\mathbf{x}| < 2R$, so that $\mu^{-1}\bar{u}R^d < c\mu^{-1}\int_{R<|\mathbf{x}|<2R} |u^*| d\mathbf{x} < c\varepsilon$, in which here and below c denotes a generic constant. It follows that

$$\begin{aligned}
\mu^{-1}\left|\int |u^*| - |u_R^*| d\mathbf{x}\right| &\leq \mu^{-1}\int_{|\mathbf{x}|<2R} \bar{u} d\mathbf{x} + \mu^{-1}\int_{|\mathbf{x}|>2R} |u^*| d\mathbf{x} \\
&\leq c\varepsilon \\
\left|\int {u^*}^2 - {u_R^*}^2 d\mathbf{x}\right| &\leq \int_{|\mathbf{x}|<2R} 2u^*\bar{u} d\mathbf{x} + \int_{|\mathbf{x}|>2R} {u^*}^2 d\mathbf{x} \\
&\leq \bar{u}\|u^*\|_1 + \varepsilon \\
&\leq c\varepsilon \\
\left|\int |\nabla u^*|^2 - |\nabla u_R^*|^2 d\mathbf{x}\right| &= \int_{|\mathbf{x}|>2R} |\nabla u^*|^2 d\mathbf{x} \\
&\leq c\varepsilon \qquad (8.19)
\end{aligned}$$

It follows that $|J[u^*] - J[u_R^*]| < c\varepsilon$ and that $|\|u^*\|_2 - \|u_r^*\|_2| < c\varepsilon$.

Define $v = a{u^*}_R$, in which a is a constant chosen so that $\|v\|_2 = 1$. It follows that $|1 - \frac{1}{a}| < c\varepsilon$, so that $|J[u^*] - J[v]| < c\varepsilon$. Since v has bounded support, Proposition 3.2 shows that $J[\psi_1] \leq J[v]$. Taking ε to 0, we get that $J[\psi_1] \leq J[u^*]$, so that $J[\psi_1] \leq J[u]$. This concludes the proof of Proposition 3.3.

9. Phase Plane Analysis in One Dimension. This appendix provides a phase plane analysis of the Euler-Lagrange equation (3.4) for dimension $d = 1$. Although the analysis is straightforward, the result is unusual because of the subgradient term in (3.4). This graphical depiction of the solution provides a geometric understanding of the formation of compact support for this ODE, which is the following:

$$\psi_{xx} - \mu^{-1}p(\psi) = -\lambda\psi \qquad (9.1)$$

in which $p(\psi)$ is the subgradient and λ and μ are both positive. This can be multiplied by ψ and integrated once to obtain

$$\psi_x^2 + \lambda(|\psi| - \lambda^{-1}\mu^{-1})^2 = \lambda^{-1}\mu^{-2} + c \qquad (9.2)$$

in which c is a constant for each orbit. The phase plane for $\lambda = \mu = 1$ is presented in Figure 9.1, along with several orbits.

The phase plane shows stationary points at $\psi = \pm(\lambda\mu)^{-1}$ corresponding to $c = -\lambda^{-1}\mu^{-2}$. Around each stationary point there are periodic orbits (for $-\lambda^{-1}\mu^{-2} < c < 0$), each of which has values that are either all positive or all negative. Away from the stationary points the orbits (for $c > 0$) are also periodic, but symmetric about $\psi = 0$. When these solutions cross $\psi = 0$, there is a discontinuity in the second derivative ψ_{xx} due to the subgradient term. In between these solutions, there are two separatrices (for $c = 0$), one nonnegative and one nonpositive. The two separatrices intersect at $(\psi, \psi_x) = (0, 0)$, which is a singular stationary point. The separatrices reach this stationary point in finite time. Note that the positive and negative periodic orbits all have the same period $2\pi\lambda^{-1/2}$, which is also the distance that each separatrix travels between its contact with the stationary point at $(0, 0)$. The period of the outer periodic solutions starts at $4\pi\lambda^{-1/2}$ close to the stationary points.

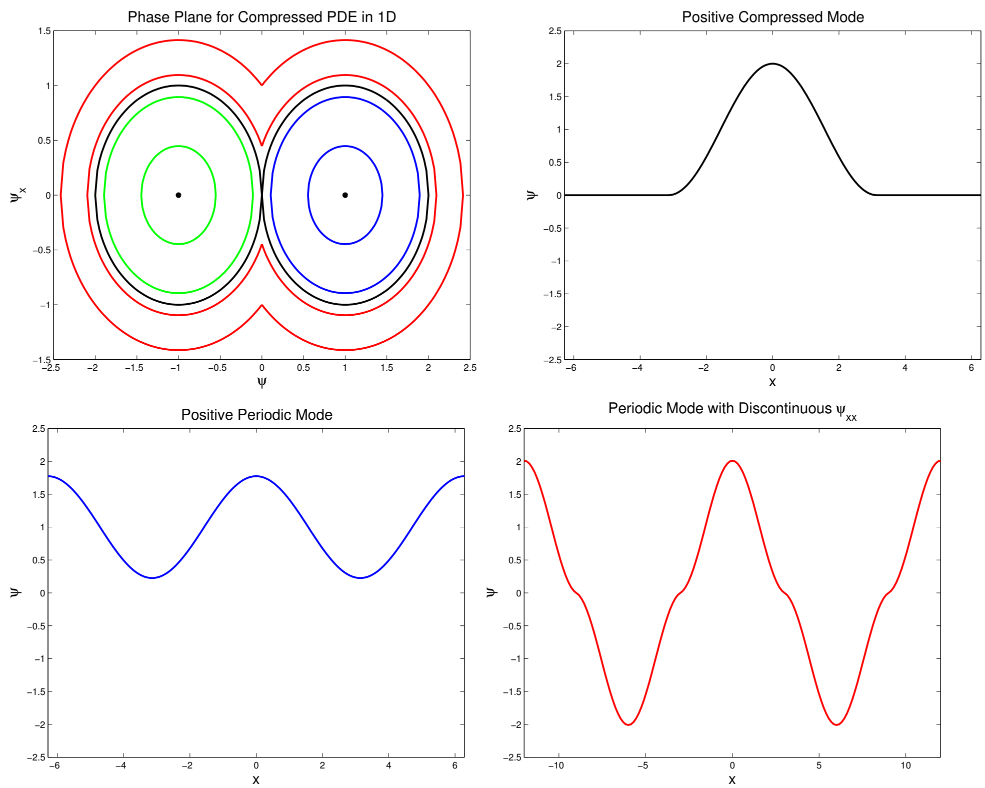

FIG. 9.1. *Solution of the Euler-Lagrange equation (9.1) in dimension* $d = 1$ *with parameters* $\lambda = \mu = 1$*. The upper left figure shows the phase plane for this solution with 8 orbits: positive and negative periodic solutions for* $c = -0.4$ *and* $c = -0.1$*, positive and negative solutions with compact support for* $c = 0$*, and periodic solution for* $c = 0.1$ *and* $c = 0.5$*. The upper right figure shows the positive solution with compact support for* $c = 0$*. The lower left figure shows the positive periodic solution for* $c = -0.2$*. The lower right figure shows the periodic solution for* $c = 0.01$*. Note that two periods are shown for each of the periodic solutions and that the vertical axes are the same in the 3 figures showing individual solutions.*