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An Analysis on Different Algorithms and Methods of Schrodinger–Poisson–Slater Equation

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Abstract – We study the existence of radially symmetric solitary waves for a non-linear Schrodinger-Poisson system. In contrast to all previous results, we consider the presence of a positive potential, of interest in physical applications.

We present a new implementation of the two-grid method for computing extremum eigenpairs of self-adjoint partial differential operators with periodic boundary conditions. A novel two-grid centered difference method is proposed for the numerical solutions of the nonlinear Schrödinger–Poisson (SP) eigenvalue problem. We solve the Poisson equation to obtain the nonlinear potential for the nonlinear Schrödinger eigenvalue problem.

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THE SCHR$\ddot{O}$DINGER-POISSON SYSTEM WITH POSITIVE POTENTIAL

In recent years great attention has been paid to some classes of systems of partial differential equations in which a Schrödinger equation is coupled to the Maxwell ones; the purpose is to describe the interaction of a nonlinear Schrödinger field with an electromagnetic field E — H. The gauge potentials $\mathbf{A} - \Phi$,

$$\mathbf{A} : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}^3, \quad \Phi : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}$$

are related to E — H by the Maxwell equations

$$\mathbf{E} \quad -\left(\nabla\Phi + \frac{\partial \mathbf{A}}{\partial t}\right), \qquad \mathbf{H} \quad \nabla \times \mathbf{A}.$$

If we are interested in finding standing waves (solutions of a field equation whose energy travels as a localized packet preserving this localization in time) and we consider the electrostatic case (when A = 0), the Schrodinger field is described by a real function $u : \mathbb{R}^3 \to \mathbb{R}$, which represents the matter (see or). In this way we are led to the following stationary system of Schrodinger- Maxwell, or Schrodinger-Poisson-Slater, type:

$$-\Delta u + \omega u - \lambda u\Phi + W_u(x, u) = 0 \qquad \text{in } \mathbb{R}^3, \tag{1}$$

$$-\Delta\Phi = u^2 \qquad \text{in } \mathbb{R}^3, \tag{2}$$

where $\omega,\ \lambda \in \mathbb{R}$ and $W : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}$ is a given potential. In particular, the second equation represents the repulsive character of the Coulomb force (the attractive case is described by the equation $\Delta\Phi = u^2$).

Such a system was studied in Benci, V., Fortunato, D. (1998) with $W \equiv 0$, and the existence of a sequence $(\omega_n, u_n, \Phi_n)_n$ of solutions was proved when the problem is settled in a bounded domain of $\mathbb{R}^3$. After that, in the potential

$$W(x, s) \quad W(s) \quad -\frac{|s|^\gamma}{\gamma}, \qquad \gamma > 2, \tag{3}$$

was introduced and existence results in the whole physical space were proved for $\gamma \in [4, 6)$, while nonexistence results for $\gamma \in (0, 2]$ or $\gamma \in [6, \infty)$ were proved in D'Aprile, T., Mugnai, D. (2004), where also more general potentials, behaving similarly to the one

in (3), were considered. In all these papers a crucial assumption is that $\lambda < 0$ and $\omega > 0$.

ince then a large number of generalizations and improvements have been produced; in particular a fundamental advance in the understanding of system (1)-(2) with W as in (3) was done in Ambrosetti, A., Ruiz, D. (2008). But also more general problems, where the first equation is replaced by

$$-\Delta u + V(x)u + u\Phi = K(x)|u|^{\gamma-2}u, \tag{4}$$

for some $V, K : \mathbb{R}^3 \to \mathbb{R},$ were studied under different assumptions on V and K; moreover, also some generalizations of the last cases, with $K(x)|u|^{\gamma-2}u$ replaced by a more generic function $f(x,u)$, were considered.

By Saanchez, O., Soler, J. (2004) a solution when *W* is as in (3) is found if $\gamma = 8/3$ and $\lambda = -1$; however, it is not known if that solution is radial. The solution is found via a minimization argument and ω appears as a Lagrange multiplier.

Let us remark that the prototype potential defined in (3), as well as all the introduced generalizations, is not always positive, while for physical reasons a potential suitable to model physical phenomena should be nonnegative: indeed, the fact that *W* is nonnegative implies that the energy density of a solution (u, $) of system (1)—(2) is nonnegative as well.

Moreover, if we consider the autonomous electrostatic case, i.e. $-\Delta u + W'(u) = 0$, calling “rest mass” of the particle u the quantity

$$\int_{\mathbb{R}^3} W(u)\,dx$$

the fact that W is positive implies that we are dealing with systems of particles having *positive mass,* which is, of course, of interest in physical applications.

Therefore, in this paper we are interested in system (1)—(2) with the main hypothesis that W is assumed *nonnegative.*

Before passing to the precise assumptions and the statement of our results, we recall that systems of this type were studied also in bounded domains both under Dirichlet or Neumann boundary conditions, and that also similar systems were treated with variational methods (as we are going to do), mainly by a suitable minimization process of the associated energy, or by critical point theory. In particular we recall that in all the papers cited before, in equation (1) the authors assume $\lambda < 0$, while for $W \equiv 0$ the case $\lambda > 0$ is treated in Lieb, E.H., Thomas, L.E. (1997), where actually is replaced by

$$-\Delta u + \omega u - 2u^2\Phi = 0 \tag{5}$$

Such an equation, also called Choquard equation, was introduced as an approximation to the Hartree-Foch theory for a one component plasma, the author proves the existence and uniqueness of a minimizing solution for the energy functional associated to a Schroodinger-Poisson problem, showing that such a minimizing solution satisfies a stationary equation of the form (5). Moreover, it is proved that such a solution is radially decreasing by Schwarz symmetrization methods. See also the recent paper, where some powers are introduced in the nonlocal part.

Let us also note that equation (1) generalizes the equation

$$-\Delta u + \omega u - u^2\Phi + \frac{5}{3}u^{7/3} = 0, \quad u > 0,$$

with $\omega > 0,$ introduced in Catto, I., Le Bris, C., Lions, P.-L. (2002) to describe a Hartree model for crystals. This equation seems to be the first example covered by our case, but in the authors were interested in *periodic* periodic structures and did not look for solutions with finite global energy, as we are going to do.

Finally, we quote Kikuchi, H. (2007), where the author studies the existence and orbital stability of standing wave solutions for system (1)—(2) when W is given in (3).

In this paper we are concerned with system (1)—(2). In all the papers just cited above in which $\lambda > 0,$, the potential W always has the form of a pure power $W(s) = |s|^\gamma/\gamma$ for some $\gamma > 2$; hence, in order to include the previous cases, in this paper we make the following assumptions:

W_1) $W : \mathbb{R}^3 \times \mathbb{R} \to [0,\infty)$ is such that the derivative $W_u : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}$ is a Caratheodory function, $W(x,s) = W(|x|,s)$ for a.e. $x \in \mathbb{R}^3$ and for every $s \in \mathbb{R}$, and $W(x,0) = W_u(x,0) = 0$ for a.e. $x \in \mathbb{R}^3$

W_2) $\exists C_1, C_2 > 0$ and $1 < q < p < 5$ such that $|W_u(x,s)| \le C_1|s|^q + C_2|s|^p$ for every $s \in \mathbb{R}$ and a.e. $x \in \mathbb{R}^3$

W_3) $\exists k \ge 2$ such that $0 \le sW_u(x,s) \le kW(x,s)$ for every $s \in \mathbb{R}$ and a.e. $x \in \mathbb{R}^3$.

Remark 1. As it will be clear from the proof, the requirement that W depends radially on the space variable is a technical assumption which lets us

reduce the problem to a radial setting. Of course, if W is independent of x, the pure power case is included in our setting and the requirement is obviously satisfied.

From Wi) we get in particular that $s = 0$ is an absolute minimum point for W for a.e. $x \in \mathbb{R}^3$, and that the system always admits the trivial solution $u = \Phi = 0$. Moreover, we remark that, by W_2) the potential W is more than quadratic both at 0 and infinity. Let us also note that by direct integration of W_3) we obtain that there exist $a, b : \mathbb{R}^3 \to [0, \infty[$ such that $W(x,s) \le a(x)|s|^k + b(x)$ for every $s \in \mathbb{R}$ and a.e. $x \in \mathbb{R}^3$, so that W may have superquadratic growth at infinity, which is in agreement with W_2). On the other hand, in W_3) we exclude the case $k < 2$, since in this latter case we would obtain that $W(x,s)/s^k$ is decreasing if $s > 0$, so that $W(x,s) \le \frac{W(x,\varepsilon)}{\varepsilon^k} s^k$ for $s > \varepsilon > 0$, and passing to the limit as $\varepsilon \to 0^+$, by W_1) we would get $W \le 0$, so that $W \equiv 0$, as it was already considered in the literature.

Remark 2. Note that our assumptions cover the case $W \equiv 0$, but even the more intriguing case in which $W(x,s) = 0$ for x belonging to a proper subset Ω of $\mathbb{R}^3$. An interesting case is when Ω is a ball, so that the potential W is active only in an exterior domain, or when Ω is an annulus. All these situations have not been considered up to now, since also in the generalizations mentioned above the coefficients V and K in (4) were assumed to be *strictly positive* in $\mathbb{R}^3$. To our best knowledge, this paper is the first one to cover the case of potentials possibly vanishing somewhere.

As usual, for physical reasons, we look for solutions that have finite energy, i.e. $(u, \Phi) \in H^1 \times D^1$, where $H^1 = H^1(\mathbb{R}^3)$ is the usual Sobolev space endowed with the scalar product

$$\langle u, v \rangle_{H^1} := \int_{\mathbb{R}^3} \left(Du \cdot Dv + uv \right) dx$$

and norm $\|u\| = (\int |Du|^2 + \int u^2)^{1/2}$, and $D^1 = D^1(\mathbb{R}^3)$ is the completion of $C_0^\infty(\mathbb{R}^3)$ with respect to the norm $\|u\|_{D^1}^2 := \int_{\mathbb{R}^3} |Du|^2 \, dx$, induced by the scalar product $\langle u, v \rangle_{D^1} := \int Du \cdot Dv \, dx$.

Before stating our main result, let us note that if $u = 0$ in (1), then $\Phi = 0$ in (2), and if $u \neq 0$, then also $\Phi \neq 0$. Therefore, we can say that a solution (u, Φ) of system (1)—(2) is *nontrivial* if both u and Φ are different from the trivial function, and a sufficient condition for this occurrence is that $u \neq 0$.

Our first result is the following easy one.

Proposition 1. *Assume that W satisfies* Wi) — W3). *Then for any* $\omega > 0$ *there exist* $\lambda > 0$ *and nontrivial radial functions* $(u, \Phi) \in H^1(\mathbb{R}^3) \times D^1(\mathbb{R}^3)$ *which solve the related system* (1) —(2).

Analogously to the previous literature, in which w was found as a Lagrange multiplier, got by a minimization process on a suitable manifold, here we find the value of λ in this way. However, in our case the manifold is different from the usual one used in the papers cited above, which adopted similar procedures considering the unit sphere in $L^2(\mathbb{R}^3)$. Indeed, we introduce a new manifold which in the end turns out to be a good choice. On the other hand, our manifold is defined as $\int u^2 \Phi = \text{constant}$, so that no rearrangement approach can be done to prove radial decreasing properties of the solutions, as done in Ruiz Arriola, E., Soler, J. (2001), where the equality $\int |u|^p = \int (u^\star)^p$ is fundamental. In fact, one could proceed as follows:

1. Prove that $u, \Phi \ge 0$;
2. Substitute u by its radial decreasing rearrangement $u^\star$ (i.e. its Schwartz symmetrization);
3. Prove that Φ is radially decreasing, so that it coincides with its decreasing rearrangement $\Phi^\star$.

Actually the last step is true for any radial function u, since Φ is radial as well and super harmonic. However, in this way the integral $\int u\Phi$ increases by the classical Hardy—Little wood inequality

$$\int_{\mathbb{R}^3} u\Phi \, dx \le \int_{\mathbb{R}^3} u^\star \Phi^\star \, dx,$$

so that a symmetrization process pushes out of the manifold under consideration.

Let us note that under assumption W_3) above, system (1)—(2) admits only the trivial solution when $\lambda \leq 0$, independently of its possible symmetry:

Proposition 2. *Assume* W_3*), and let* $(u, \Phi) \in H^1(\mathbb{R}^3) \times D^1(\mathbb{R}^3)$ *be a solution of system* (1) —(2) *with* $\lambda \leq 0$. *Then* $u = \Phi = 0$

Proof. Multiplying and integrating parts, W_3) gives

$$0 = \int_{\mathbb{R}^3} |Du|^2\,dx + \omega \int_{\mathbb{R}^3} u^2\,dx - \lambda \int_{\mathbb{R}^3} u^2\Phi\,dx + \int_{\mathbb{R}^3} W_u(x,u)u\,dx$$
$$\geq \int_{\mathbb{R}^3} |Du|^2\,dx + \omega \int_{\mathbb{R}^3} u^2\,dx;$$

since $\omega > 0$. This implies $u \equiv 0$, as claimed. By (2) we immediately get $\Phi = 0$.

Thus, if W_3) holds, it is natural to look for solutions when $\lambda > 0$, as stated in Theorem 1.

On the other hand, the importance of radial functions, and in particular of positive ones, has been widely used in open quantum problems, and in addition they provide a more friendly functional setting from a mathematical point of view.

On the other hand, from a physical viewpoint, positive solutions are the most natural ones, and in fact. *Under the assumptions of Proposition* 1, *the solution u of* (1) *is strictly positive in* $\mathbb{R}^3$.

We remark that the fact that Φ is positive is a free result, since by direct integration of (2) we get

$$\Phi(x) = \int_{\mathbb{R}^3} \frac{1}{4\pi|x-y|} u^2(y)dy, \tag{6}$$

so that $\Phi > 0$, as soon as $u \neq 0$.

Variational techniques can improve the existence result above when W satisfies some symmetry conditions. In this way we get the two main results of this paper, collected in the theorems below.

Theorem 1. *Under the assumptions of Proposition* 1, *let us also assume that* $W(x,s) = W(x,-s)$ *for* $a.e.\ x \in \mathbb{R}^3$ *and every* $s \in \mathbb{R}$. *Then for every* $\omega > 0$ *there exist infinitely many triples* $(\lambda, u, \Phi) \in \mathbb{R}^+ \times H^1(\mathbb{R}^3) \times D^1(\mathbb{R}^3)$ *which solve the related system* (1) —(2).

The main fact in the previous results is that λ is not given *a priori*, but is found as a Lagrange multiplier. However, if we let p vary in a smaller set, then λ can be fixed from the very beginning, thus improving the result of Proposition 1 in the following way:

Theorem 2. *Assume that W satisfies* W_1*),* W_2*) with* $p \in (1,3)$ *and* W_3*) with* $k \leq 4$. *Then for any* $\lambda, \omega > 0$ *there exist nontrivial radial functions* $(u, \Phi) \in H^1(\mathbb{R}^3) \times D^1(\mathbb{R}^3)$ *which solve* (1)-(2).

The fact that in Theorem 2 p is not too large lets us employ classical variational techniques, such as the Mountain Pass Theorem, which could not be applied to prove Theorem 1, since the geometric conditions of the latter theorem fail if $p \geq 3$.

EFFICIENT ALGORITHM FOR THE SCHRÖDINGER–POISSON EIGENVALUE PROBLEM

In recent years, some numerical methods have been proposed for computing the first few eigenpairs of the Schrodinger eigenvalue problem. In particular, the homotopy continuation method was exploited to solve the Schrodinger eigenvalue problem with Dirichlet boundary conditions, where various linear potentials were numerically tested. However, in the case of Dirichlet boundary conditions most of the multiple eigenvalues are double. Livne and Brandt design linear-complexity multiscale algorithms for computing, storing, and manipulating eigenfunctions of the 1D periodic Schrodinger eigenvalue problem and other related differential operators. Recent research articles concerning the computations of interior eigenpairs of the Schrodinger equation can be found in.

Xu and Zhou(1999) developed a two-grid finite element discretization scheme for second order linear elliptic eigenvalue problems. Let $\tilde{h}$ and h be the uniform meshsizes on the coarse and the fine grids, and (u, λ) and (u_h, λ_h) be the corresponding exact and the approximate eigenpairs on the fine grid, respectively. They show that $\|\nabla(u - u_h)\|_{L^2} = O(h + \tilde{h}^2)$ and $|\lambda - \lambda_h| = O(h^2 + \tilde{h}^4)$. These estimates mean that one can obtain asymptotic optimal errors by taking $\tilde{h} = O(h^{\frac{1}{2}})$. Recently the authors developed a two-grid finite element discretization scheme for semilinear elliptic eigenvalue problems.

In this paper we modify the two-grid finite element scheme in. and propose a new' implementation of the two- grid method for computing extremum eigenpairs of self-adjoint partial differential operators with periodic boundary conditions. The problem can be expressed as

$$F(u, \lambda) = 0, \tag{7}$$

where $F : \mathbf{B} \times \mathbb{R} \to \mathbf{B}$ is a smooth mapping with $u \in \mathbf{B}$, $\lambda \in \mathbb{R}$, $\mathbf{B}$ is some Banach space, and $\mathbb{R}$ is the real line. For the Schrodinger eigenvalue problem

$$L(\phi, \omega) = -\Delta\phi + \widetilde{V}\phi - \omega\phi = 0, \tag{8}$$

where $(\phi, \omega) = (0, \omega)$ is a trivial solution, where $\widetilde{V}$ is the linear potential. Therefore, we can treat an eigenpair of the operator equation as a solution curve branching from the trivial solution curve at the eigenvalue. We will combine the ideas of the two-grid discretization scheme together with the predictor-corrector method and develop a new algorithm for computing the extremum eigenpairs of the discrete Schrodinger eigenvalue problem.

To start, we discretize the operator equation (7) on the coarse grid by the centered difference approximations. Then we use the block Lanczos method to compute extremum eigenpairs on the coarse grid, which also can handle multiple and clustered eigenpairs as well. The implementations are inexpensive since the order of the coefficient matrix on the coarse grid is relatively small compared to the one on the fine grid. An alternative is to use the function eig in Matlab to compute the first few eigenpairs. The extremum eigenpairs we obtained on the coarse grid will be used as predicted model of extremely small devices in semiconductor nanostructures where the quantum structure has to be taken into account. We also use the block Lanczos method to compute the first few, say k eigenpairs on the coarse grid. Then we consider the nonlinear Schrodinger eigenvalue problem as a parameter-dependent problem

$$L(\phi, \omega) + \alpha N(\phi) = 0, \quad \alpha \in [0, 1], \tag{9}$$

where $N(\phi) = V\phi$ denotes the effect of the nonlinear potential V. We choose an initial step size ao with $j\alpha_0 = 1, \quad j \in \mathbb{N},$ for the continuation method, and solve the Poisson equation to obtain V for (9). Then we go back to (9) and use the block Lanczos method to find the first k eigenpairs. This process is repeated until $j\alpha_0 = 1$ is reached.

In addition, the eigenpairs are updated until they converge. We also use the eigenpairs obtained on the coarse grid as initial guesses for computing their counterparts on the line grid. Moreover, the RQI is also exploited to improve the accuracy of the approximate eigenpairs. Our method can be easily modified to compute numerical solutions of the Schrodinger-Poisson-Slater (SPS) system. Numerical study of the SP system can be found.

The analysis is based on the performance of the proposed method with the linear eigenvalue problem as the test problem, where the discrete eigenpairs are available. Moreover, we also discuss the group actions on the basis functions of the eigenspace in the presence of symmetry. Our numerical results show that the convergence rate of eigenvalue computations on the fine grid is O(h^3). Moreover, one RQI makes the first few eigenvalues of the linear eigenvalue problem correct at least up to eleven decimal digits. In this Section we derive a two-grid centered difference method for computing the first few eigenpairs of the Schrodinger-Poisson eigenvalue problem (ESP). Our numerical results show that: (i) a cluster of eigenvalues can be computed completely on the fine grid, (ii) separation of eigenvectors on the coarse grid is preserved on the fine grid, (iii) eigenvalues in different clusters can be treated simultaneously. Our numerical results show how the first few eigenpairs of the Schrodinger eigenvalue problem are affected by the dopant which is considered in the SP system.

A two-grid discretization method-

Bifurcation from multiple and clustered eigenvalues - Let B be a Banach space of smooth functions endowed with some norm, and $\mathbb{R}$ the set of all real numbers. We treat the Schrodinger eigenvalue problem as a parameter-dependent operator equation of the following form

$$F(u, \lambda) := -\Delta u + fu - \lambda u = 0 \quad \text{in } \Omega = [0, a]^n, \tag{10}$$

where $F : \mathbf{B} \times \mathbb{R} \to \mathbf{B}$ is a smooth mapping with $u \in \mathbf{B}$, $\lambda \in \mathbb{R}$, $n = 2$ or 3, and/is a function of spatial variables which is properly chosen so that the operator $(-\Delta + fI)$ is self-adjoint. Here I denotes the identity operator on B.

We may impose Dirichlet or periodic boundary conditions on $\partial\Omega$. Choosing periodic boundary conditions will increase the multiplicity of eigenvalues. Besides, it is consistent with the real situation in quantum physics. Both boundary conditions were imposed on (10) in our numerical experiments. But our numerical reports are mainly concerned with on the latter.

It is well known if the spectrum $\sigma(A)$ of the coefficient matrix A is simple, then the Gauss-Newton method and its many improved modifications can be applied for solving $Ax = \lambda x$. However, the Gauss-Newton method converges only to one zero at a time if it converges. Li and his collaborators studied homotopy continuation methods for computing eigenpairs of large sparse eigenproblems. where the coefficient matrix can be symmetric or nonsymmetric. Lui and

Golub also studied homotopy method for (10). The two-grid method we propose here can compute both multiple and clustered eigenvalues. Moreover, a cluster of eigenvalues on the fine grid can be computed completely, and eigenvalues in different clusters can be treated simultaneously.

Note that $(0, \lambda)$ is a trivial solution of (10) for all $\lambda \in \mathbb{R}$. Moreover, (u^*, λ^*) is an eigenpair of (10) if and only if $_{x}$, $F(u^*, \lambda^*) = 0.$, Thus, $(0, \lambda^*)$ is a bifurcation point on the trivial solution curve $\{(0, \lambda) \mid \lambda \in \mathbb{R}\}$. The bifurcation diagram of (10) is similar to that. One may use the predictor-corrector continuation method described to trace the first few numerical solution branches of (10) bifurcating at eigenvalues, including multiple and clustered eigenvalues. However, our aim here is computing extremum eigenpairs of the discrete Schrodinger eigenvalue problem rather than tracing its solution curves, which are of little interest because they are lines that are perpendicular to the trivial solution curve.

Derivation of the algorithm - Let $\tilde{h} = a/\tilde{N}$ and $h = a/N$ be chosen so that $\tilde{h}, h \in (0, 1)$, where $\tilde{N}$ and N are positive integers. Suppose that (10) is discretized by the centered difference approximations with uniform meshsizes. Let $F_{\tilde{h}}$ and F_h be the discrete operators corresponding to (10) on the coarse grid $\Omega^{\tilde{h}}$ and tine grid Ω^h, respectively. Without loss of generality, we consider periodic boundary conditions. Since our purpose is to compute extremum eigenpairs of the discrete Schrodinger eigenvalue problem, it is more realistic to consider the discrete operators associated with (10). namely,

$$F_{\tilde{h}}(u, \lambda) = (A_{\tilde{h}} + D_{\tilde{h}} - \lambda I)u = 0 \tag{11}$$

and

$$F_h(u, \lambda) = (A_h + D_h - \lambda I)u = 0. \tag{12}$$

Both (11) and (12) are nonlinear systems of equations, where $F_{\tilde{h}} : \mathbb{R}^{\tilde{N}^n} \times \mathbb{R} \to \mathbb{R}^{\tilde{N}^n}$ $F_h : \mathbb{R}^{N^n} \times \mathbb{R} \to \mathbb{R}^{N^n}$ $A_{\tilde{h}} \in \mathbb{R}^{\tilde{N}^n \times \tilde{N}^n}$ and $A_h \in \mathbb{R}^{N^n \times N^n}$ are the coefficient matrices corresponding to the Laplace operator $-\Delta$ on the coarse and fine grids, and $D_{\tilde{h}} \in \mathbb{R}^{\tilde{N}^n \times \tilde{N}^n}$ and $D_h \in \mathbb{R}^{N^n \times N^n}$ are diagonal matrices whose diagonal entries are the values off at each coarse and fine grid points, respectively. We will discuss how the extremum eigenpairs, including both multiple and clustered eigenpairs on the fine grid, can be approximated by their counterparts on the coarse grid.

The matrix eigenvalue problem corresponding to (11) on the coarse grid can be expressed as

$$B_{\tilde{h}} u_{\tilde{h}} = \lambda_{\tilde{h}} u_{\tilde{h}}, \tag{13}$$

where $B_{\tilde{h}} = A_{\tilde{h}} + D_{\tilde{h}}$. Note that the coefficient matrix $B_{\tilde{h}}$ in (13) is symmetric positive definite. We apply the block Lanczos method to compute, say. the first k eigenpairs of (13). which are denoted by $(\bar{u}_{\tilde{h}}, \bar{\lambda}_{\tilde{h}})$. Alternatively, one can also use the function eig in Matlab to compute eigenpairs on the coarse grid.

Theorem 3. Let $B_h = A_h + D_h$ and assume that $(\bar{u}_{\tilde{h}}, \bar{\lambda}_{\tilde{h}})$ can be used as an initial guess in Newton's method for approximating the zero point (u_h, λ_h) of $F_h(u, \lambda) = 0$ on the fine grid. Then the eigenvector u_h on the fine grid is obtained by solving

$$B_h u_h = \bar{\lambda}_{\tilde{h}} (I_{\tilde{h}}^h \bar{u}_{\tilde{h}}), \tag{14}$$

where $I_{\tilde{h}}^h : \Omega^{\tilde{h}} \to \Omega^h$ is an interpolation operator yet to be specified.

Proof. Consider the first order Taylor expansion of the mapping $F_h(u, \lambda)$ at $(I_{\tilde{h}}^h \bar{u}_{\tilde{h}}, \bar{\lambda}_{\tilde{h}})$. namely,

$$F_h(u, \lambda) = F_h(I_{\tilde{h}}^h \bar{u}_{\tilde{h}}, \bar{\lambda}_{\tilde{h}}) + D_u F_h(I_{\tilde{h}}^h \bar{u}_{\tilde{h}}, \bar{\lambda}_{\tilde{h}})(u - I_{\tilde{h}}^h \bar{u}_{\tilde{h}}) + D_\lambda F_h(I_{\tilde{h}}^h \bar{u}_{\tilde{h}}, \bar{\lambda}_{\tilde{h}})(\lambda - \bar{\lambda}_{\tilde{h}}) + O(\|u - I_{\tilde{h}}^h \bar{u}_{\tilde{h}}\|^2 + |\lambda - \bar{\lambda}_{\tilde{h}}|^2). \tag{15}$$

Denote the differential of F_h by $DF_h = [D_u F_h, D_\lambda F_h]$, where $D_u F_h = (A_h + D_h - \lambda I) \in \mathbb{R}^{N^n \times N^n}$ and $D_\lambda F_h = -u \in \mathbb{R}^{N^n}$. If (u, λ) is replaced by (u_h, λ_h) and if we neglect the error term in (9), we get

$$-F_h(I_{\tilde{h}}^h \bar{u}_{\tilde{h}}, \bar{\lambda}_{\tilde{h}}) \approx (A_h + D_h - \bar{\lambda}_{\tilde{h}} I)(u_h - I_{\tilde{h}}^h \bar{u}_{\tilde{h}}) - I_{\tilde{h}}^h \bar{u}_{\tilde{h}} (\lambda_h - \bar{\lambda}_{\tilde{h}})$$

which implies that

$$-(A_h + D_h) I_{\tilde{h}}^h \bar{u}_{\tilde{h}} + \bar{\lambda}_{\tilde{h}} (I_{\tilde{h}}^h \bar{u}_{\tilde{h}}) \approx (A_h + D_h - \bar{\lambda}_{\tilde{h}} I)(u_h - I_{\tilde{h}}^h \bar{u}_{\tilde{h}}) - I_{\tilde{h}}^h \bar{u}_{\tilde{h}} (\lambda_h - \bar{\lambda}_{\tilde{h}})$$

After simple calculations we obtain

$$B_h u_h \approx \bar{\lambda}_{\tilde{h}} (I_{\tilde{h}}^h \bar{u}_{\tilde{h}}). \tag{16}$$

Note that the vector $I_{\tilde{h}}^h \bar{u}_{\tilde{h}}$ in (16) must be treated as a vector on the fine grid. Eq. (16) shows that we can get an approximate eigenvector $\bar{u}_h$ corresponding to the exact eigenvector n/, on Ω^h by solving (14).

We chose $I_{\tilde{h}}^{h}$ as the linear interpolation in our numerical experiments. The process we described above belongs to the class of one-step linearization methods, which actually is the Newton method. Theorem 3 shows that performing the first Newton iteration on the fine grid is equivalent to solving (14) there.

Suppose that we already obtained the first k approximate eigenpairs on the coarse grid $\Omega^{\tilde{h}}$. To compute the corresponding approximate eigenpairs on the fine grid, we propose to use the CG method to solve (14), namely, k SPD linear systems only a few iterations. For consistence with the RQI solver, we also use MINRES to solve (14). Our main concern here is that the fine grid solutions only serve as starting initial guesses for the RQI. Clearly, if $\bar{u}_h$ is an approximate eigenvector on the fine grid, the Rayleigh quotient of $\bar{u}_h$ is a reasonable choice for the corresponding eigenvalue $\bar{\lambda}_h$ To obtain the fine grid approximate eigenvalue $\bar{\lambda}_h$, we compute the Rayleigh quotient

$$\bar{\lambda}_h = \frac{\bar{u}_h^{\mathrm{T}} B_h \bar{u}_h}{\bar{u}_h^{\mathrm{T}} \bar{u}_h}.$$

On the other hand, if $\bar{\lambda}_h$ is an approximate eigenvalue on the fine grid, then from the inverse power method one sees that thesolution to $(B_h - \bar{\lambda}_h I)x = \bar{u}_h$ will be a good approximate eigenvector. Combining these two ideas together, we use $(\bar{u}_h, \bar{\lambda}_h)$ as an initial guess, and perform the RQI on the fine grid. In Parlett has shown that the RQI converges globally and that the rate of convergence is ultimately cubic. Thus, performing RQI on the fine grid will efficiently improve the accuracy of the computed eigenpairs. Since the condition number of the coefficient matrix increases as the approximate eigenvalue approaches the exact one. we exploit the technique described in which we briefly describe as follows:

Suppose that (u_1, λ_1) is an eigenpair of a symmetric matrix A. and (u_0, λ_0) is an approximation to (u_1, λ_1). Instead of solving

$$(A - \lambda_0 I)y = u_0, \tag{17}$$

we solve a rank-one modification of the coefficient matrix $A - \lambda_0 I$, i.e.,

$$(A - \lambda_0 I + u_0 u_0^{\mathrm{T}})z = u_0.$$

Then we have

$$(A - \lambda_0 I)z = (1 - u_0^{\mathrm{T}} z)u_0.$$

Thus the solution of (11) is $y = z/(1 - u_0^{\mathrm{T}} z)$. Our numerical results show that the technique can be used to handle both simple and multiple eigenvalues. Based on the results, we used the MINRES 1211 to solve linear systems in the RQI.

In summary, the procedure we described above for computing the extremum eigenpairs of (10) can be regarded as a predictor-corrector method. In the predictor step, we compute the extremum eigenpairs of the discrete operator equation on the coarse grid, which are used as initial guesses for computing the counterparts on the fine grid. In the corrector step, we solve (14) and perform the RQI. There is no continuation because the solution curves go straight.

CONCLUSION

The existence of positive solutions to Schrodinger–Poisson type systems in $\mathbb{R}^3$ with critically growing nonlocal term is proved by using variational method which does not require usual compactness conditions.

We present an efficient algorithm, for computing the extremum eigenpairs of the Schrödinger eigenvalue problem. The convergence rate of eigenvalue computations on the fine grid is O(h^3). Moreover, one RQI makes the first few approximate eigenvalues of the linear eigenvalue problem correct up to eleven decimal digits.

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