COMPUTING THE GROUND STATE AND DYNAMICS OF THE SCHRÖDINGER EQUATION WITH NONLOCAL POTENTIALS VIA NONUNIFORM FFT

WEIZHU BAO *, SHIDONG JIANG †, QINGLIN TANG ‡, AND YONG ZHANG §

Abstract. We present a novel efficient and accurate solver for computing the ground state and dynamics of the Schrödinger-Poisson equation via nonuniform FFT (NUFFT). We first extend the algorithm developed in [21] to compute the 2D Coulomb interactions via NUFFT. We then incorporate these spectrally accurate algorithms into the solver for computing the ground state and dynamics of the Schrödinger-Poisson equation. Combined with the gradient flow method for the ground state and the time splitting method for the dynamics, our new solver is much more accurate as compared with existing solvers. A detailed and systematic comparative study of the new method with the existing scheme has been carried out, and the results are demonstrated with several numerical examples.

Key words. nonlinear Schrödinger equation, Poisson equation, fractional Poisson equation, nonuniform FFT

1. Introduction. The Schrödinger-Poisson system (SPS), derived from the N-body quantum system with Hartree ansatz for electron wavefunction, is of great importance in semiconductor device. The electron-electron interactions are usually modelled by the Coulomb potential in three dimensions. However, for many physical systems, the electrons are confined to a two dimensional plane, and their interactions are described via the fractional Poisson equation in two dimensions. There are also physical systems where the distribution of the electrons are uniform in one direction, say, the z direction. In this case, the interactions are described via the Poisson equation in two dimensions.

To summarise, we consider the Schrödinger equation, in dimensionless form, with Coulomb interactions as follows:

$$i\,\partial_t\psi(\mathbf{x},t) = \left[-\frac{1}{2}\Delta + V(\mathbf{x}) + \beta\,\varphi\right]\psi, \qquad \mathbf{x}\in\mathbb{R}^d, \quad t>0, \tag{1.1}$$

$$\varphi(\mathbf{x},t) = \left(U * |\psi|^2\right)(\mathbf{x},t), \qquad \mathbf{x}\in\mathbb{R}^d, \quad t\geq 0, \tag{1.2}$$

$$\psi(\mathbf{x},t=0) = \psi_0(\mathbf{x}), \qquad \mathbf{x}\in\mathbb{R}^d. \tag{1.3}$$

Here, $\psi(\mathbf{x},t)$ is the complex-valued wavefunction, $V(\mathbf{x})$ is the external potential, β is the coupling constant (positive for repulsive interaction and negative for attractive interaction), and the real-valued function $\varphi(\mathbf{x},t)$ is the Coulomb potential given by the convolution of the kernel U and the charge density $\rho := |\psi|^2$. The convolution

*Department of Mathematics and Center for Computational Science and Engineering, National University of Singapore, Singapore 119076, (bao@math.nus.edu.sg (W. Bao)).

†Department of Mathematical Sciences, New Jersey Institute of Technology, Newark, New Jersey, 07102 (shidong.jiang@njit.edu). This research was supported by the National Science Foundation under grant CCF-0905395.

‡Wolfgang Pauli Institute c/o Fak. Mathematik, University Wien, Oskar-Morgenstern-Platz 1, 1090 Vienna, Austria. sunny5zhang@gmail.com (Y. Zhang); tqltql2010@gmail.com (Q. Tang).

kernel U is given explicitly by the following formula

(1.4)
$$U(\mathbf{x}) = \begin{cases} -\frac{1}{2\pi}\ln|\mathbf{x}|, & \mathbf{x}\in\mathbb{R}^2 \\ \frac{1}{2\pi|\mathbf{x}|}, & \mathbf{x}\in\mathbb{R}^2 \\ \frac{1}{4\pi}|\mathbf{x}|^{-1}, & \mathbf{x}\in\mathbb{R}^3 \end{cases} \Longleftrightarrow \widehat{U}(\xi) = \begin{cases} \frac{1}{2\pi}\,\frac{1}{|\xi|^2}, & \xi\in\mathbb{R}^2, \quad \text{2D SPS} \\ \frac{1}{|\xi|}, & \xi\in\mathbb{R}^2, \quad \text{2.5D SPS} \\ \frac{1}{(2\pi)^{3/2}}\,\frac{1}{|\xi|^2}, & \xi\in\mathbb{R}^3, \quad \text{3D SPS} \end{cases}$$

where $\widehat{U}(\xi) = \frac{1}{(2\pi)^{d/2}}\int_{\mathbb{R}^d} U(\mathbf{x})\, e^{-i\xi\cdot\mathbf{x}}\mathrm{d}\mathbf{x}$ is the Fourier transform of $U(\mathbf{x})$, $\mathbf{x},\xi\in\mathbb{R}^d$.

The existence and uniqueness of the ground state of the Schrödinger-Poisson system has been shown in []. The numerical study of ground state of the SPS has been carried out in []. Due to the nonlinearity of the SPS, the ground state is often computed via the backward Euler method to solve the time-dependent problem with a suitably chosen initial state (see, for example, []). The dynamics of the SPS has also been studied extensively. Indeed, for the well-posedness of the Cauchy problem for the SPS, we refer to [11, 13, 23, 24]. And the numerical study of the dynamics of the SPS can be found in []. Here the standard time marching scheme is the so-called time-splitting method (see, for example, []). In both cases, the wave function decays rapidly in space and the spatial computation domain is often truncated to a rectangular box. The accuracy of the numerical method in the spatial variable is dominated by the evaluation of the nonlocal interaction potential ϕ.

Currently, the most popular method of evaluating the Coulomb interactions is to solve the associated partial differential equation on the truncated rectangular box with either periodic or homogeneous Dirichlet boundary condition imposed on the boundary. Indeed, it is easy to see that the nonlocal potential ϕ satisfies the Poisson equation for 2D and 3D SPS

$$-\Delta\,\varphi(\mathbf{x},t) = |\psi(\mathbf{x},t)|^2, \qquad \mathbf{x}\in\mathbb{R}^d,\ d=2,3; \tag{1.5}$$

and the fractional Poisson equation for 2.5D SPS,

$$\sqrt{-\Delta}\,\varphi(\mathbf{x},t) = |\psi(\mathbf{x},t)|^2, \quad \mathbf{x}\in\mathbb{R}^2. \tag{1.6}$$

When the periodic boundary condition is posed on the boundary, the FFT is often used to compute the potential. However, the zeroth mode of the Fourier series is incorrectly set to zero since the Laplacian operator has the symbol $|\xi|^2$. This causes the so-called "numerical locking" phenomena and the overall accuracy of the potential evaluation is thus not high when the total charge of the physical system is not zero. On the other hand, when the homogeneous Dirichlet condition is imposed, the discrete sine transform (DST) is often used since the solution can be expressed as a sine series in this case. The Fourier modes near the origin are again not well resolved for the DST method even though the "numerical locking" phenomena are less severe since the DST method avoids the zeroth mode altogether.

Obviously, both the FFT method and the DST method result in low accuracy for the potential evaluation since the Coulomb interactions are nonlocal and long range and neither periodic boundary condition nor the homogeneous boundary condition is correct at the boundary of the truncated rectangular box. For 2.5D and 3D Schrödinger-Poisson systems, the DST method can gain some accuracy by enlarging the computational domain since the potential decays like $1/r$. But because the decaying rate is very slow, the increase in the accuracy is achieved at the expense of rapidly growing computational cost.

The situation becomes much worse for the 2D Schrödinger-Poisson system. Indeed, the 2D Coulomb potential increases logarithmically if the total charge of the physical system is not zero. Thus the homogeneous boundary condition is essentially wrong and the DST suffers from huge loss of accuracy no matter how large the computational domain is. The FFT method suffers from the "numerical locking" phenomenon as before.

Recently, an efficient and accurate algorithm is developed in [21] to compute the Coulomb interactions in 2.5 and 3 dimensions. The algorithm starts from the Fourier integral representation of the Coulomb potential, discretize the Fourier integral using high-order quadratures in either the polar coordinates or spherical coordinates, and then evaluates the resulting discrete summation using the nonuniform FFT. The algorithm has $O(N \log N)$ complexity and is spectrally accurate for smooth densities.

In this paper, we first extend the algorithm in [21] to compute the Coulomb interaction in two dimensions. We note first that the Fourier integral representation of the Coulomb potential actually diverges at the origin when the total charge of the physical system is nonzero and thus can not be used directly. Our method is to split the potential into two parts $\phi = \phi_1 + \phi_2$. The first part ϕ_1 is induced by a smooth Gaussian whose total charge is equal to that of the original system. And the second part ϕ_2 is induced by a charge density whose total charge is zero and whose smoothness and decaying property are the same as before. We then show that ϕ_1 has an analytical expression. Obviously, ϕ_2 now has a well-defined Fourier integral representation and thus can be computed efficiently and accurately using the algorithm in [21].

REMARK 1.1. *When the density function has complicated local structure, an adaptive grid is more efficient and some other fast algorithms such as the fast multipole method may be applied to evaluate the potentials in this case. We also note that recently Zhang et. al. [25] derived exact artificial boundary conditions for the 2D Poisson equation (1.5) on a disk. They used the FFT for the azimuthal direction and a second order finite scheme to solve each Fourier mode in r direction. The resulting method is second order in space.*

We then incorporate our NUFFT based algorithm for the evaluation of the nonlocal potentials into the solvers for computing the ground state and dynamics of the SPS in 2, 2.5, and 3 dimensions. A systematic comparison of our new method with the existing methods has been carried out and the results show that our new method performs much better than the existing methods. To be more precise, our new method requires smaller spatial computational domain and coarser mesh to achieve higher precisoin as compared with the existing methods.

This paper is organized as follows. In Section 2, we briefly review the algorithm in [21] for evaluating the Coulomb potentials in 2.5 and 3 dimensions, and describe in detail the method for computing the Coulomb potential in two dimensions. In Section 3, a comparative study for computing the ground state of the SPS is presented. And in Section 4, we show the numerical results for the dynamics of the SPS. Finally, we conclude the paper in Section 5.

2. Evaluation of the nonlocal potentials. In this section, we present an efficient and accurate algorithm for evaluating the Coulomb interaction in two dimensions. We first review briefly the algorithms for evaluating the Coulomb interactions in 2.5 and 3 dimensions via NUFFT. For details, please see [21].

2.1. Evaluation of the Coulomb interactions in 2.5 and 3 dimensions. In the Fourier space, the Coulomb interactions in 2.5 and 3 dimensions have the following

expression:

$$\varphi(\mathbf{x}) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{i\,\mathbf{k}\cdot\mathbf{x}}\, \widehat{U}(\mathbf{k})\, \widehat{\rho}(\mathbf{k})\, d\mathbf{k}, \qquad \mathbf{x} \in \mathbb{R}^d, \qquad d = 2, 3, \tag{2.1}$$

where $\widehat{U}(\mathbf{k})$ is given by one of the formulae

$$\widehat{U}(\mathbf{k}) = \begin{cases} \dfrac{1}{|\mathbf{k}|^2}, & d = 3, \ \text{3D Coulomb interactions}, \\ \dfrac{1}{|\mathbf{k}|}, & d = 2, \ \text{2.5D Coulomb interactions}. \end{cases} \tag{2.2}$$

In both cases, it is easy to see that the singularities at the origin can be removed by a coordinate trasform to spherical and polar coordinates, respectively. Thus, the above integral can be discretized using high order quadratures and the resulting summation can be evaluated using NUFFT. This leads to an $O(N \log N)+O(M)$ algorithm where N is the number of equispaced points in the physical space and M is the number of nonequispaced point in the Fourier space. However, M is roughly N and the constant in front of $O(M)$ is much greater than the constant in front of $O(N \log N)$, which makes the algorithm slower than the regular FFT by a large factor, especially for three dimensional problems.

In order to reduce the interpolation cost in NUFFT, the integral in (2.1) is splitted into two parts using a simple partition of unity.

$$\begin{aligned} \varphi(\mathbf{x}) &\approx \frac{1}{(2\pi)^d} \int_{|\mathbf{k}|\le P} e^{i\mathbf{k}\cdot\mathbf{x}} \widehat{U}(\mathbf{k}) \widehat{\rho}(\mathbf{k}) d\mathbf{k} \\ &= \int_{|\mathbf{k}|\le P} e^{i\mathbf{k}\cdot\mathbf{x}} \frac{\widehat{U}(\mathbf{k})}{(2\pi)^d} \widehat{\rho}(\mathbf{k})(1 - p_d(\mathbf{k})) d\mathbf{k} + \int_{|\mathbf{k}|\le P} e^{i\mathbf{k}\cdot\mathbf{x}} \frac{\widehat{U}(\mathbf{k})}{(2\pi)^d} \widehat{\rho}(\mathbf{k}) p_d(\mathbf{k}) d\mathbf{k} \\ &:= I_1 + I_2. \end{aligned} \tag{2.3}$$

The function p_d is chosen to be a monotone C^∞ function which decays rapidly, and such that $\frac{1-p_d(\mathbf{k})}{|\mathbf{k}|^{d-1}}$ is a smooth function for $\mathbf{k} \in \mathbb{R}^d$. With this choice of p_d, I_1 can be computed using the regular FFT and I_2 can be computed using the NUFFT with a fixed number of irregular points in the Fourier space. Thus the interpolation cost in NUFFT is reduced to $O(1)$ and the cost of the overall algorithm is comparable with that of the regular FFT, with an oversampling factor (2^3 for 3D problems and $2^2 - 3^2$ for 2D problems) in front of $O(N \log N)$.

2.2. Evaluation of the Coulomb interaction in 2D. We now consider the evaluation of the Coulomb interactions in two dimensions. That is, we try to solve the free space Poisson equation in two dimensions:

$$-\Delta\varphi(\mathbf{x}) = \rho(\mathbf{x}). \tag{2.4}$$

The difficulty associated with this problem is that the solution does not decay to zero at infinity. Instead, the physically meaningful solution approaches $-\frac{Q}{2\pi} \ln(|\mathbf{x}|)$ as $\mathbf{x} \to \infty$, where $Q = 2\pi\, \widehat{\rho}(\mathbf{0}) = \int_{\mathrm{R}^2} \rho(\mathbf{x}) \mathrm{d}\mathbf{x}$ is the total charge in the system. And the Fourier integral representation of the solution

$$\varphi(\mathbf{x}) = \frac{1}{2\pi} \int_{\mathbb{R}^2} \frac{\widehat{\rho}(\mathbf{k})}{|\mathbf{k}|^2}\, e^{\,i\,\mathbf{k}\cdot\mathbf{x}}\, \mathrm{d}\mathbf{k}, \quad \mathbf{x} \in \mathbb{R}^2, \tag{2.5}$$

actually diverges due to the singularity at the origin when the total charge Q is nonzero.

REMARK 2.1. *We would like to remark that any derivative of the solution has well defined Fourier integral representation and thus can be evaluated accurately and efficiently using the algorithms in [21].*

We now split the solution as follows:

$$\varphi(\mathbf{x}) := \varphi_1(\mathbf{x}) + \varphi_2(\mathbf{x}), \tag{2.6}$$

where φ_1 and φ_2 are the solutions to the following equations:

$$-\Delta\varphi_1(\mathbf{x}) = \widehat{\rho}(\mathbf{0})\frac{\sigma^2}{2}\, e^{-\frac{1}{4}\sigma^2|\mathbf{x}|^2}, \tag{2.7}$$

$$-\Delta\varphi_2(\mathbf{x}) = \rho(\mathbf{x}) - \widehat{\rho}(\mathbf{0})\frac{\sigma^2}{2}\, e^{-\frac{1}{4}\sigma^2|\mathbf{x}|^2}. \tag{2.8}$$

Here σ is a parameter to be chosen shortly. We first observe that φ_1 satisfies the following far field condition at infinity

$$\varphi_1(\mathbf{x}) \to -\widehat{\rho}(\mathbf{0})\ln(|\mathbf{x}|), \qquad \mathbf{x}\to\infty. \tag{2.9}$$

Notice that φ_1 is also radially symmetric and thus is a function of $r = |\mathbf{x}|$ only. In this case, the Poisson equation is reduced to a second order ODE:

$$-\frac{1}{r}\partial_r(r\partial_r\varphi_1) = \widehat{\rho}(\mathbf{0})\frac{\sigma^2}{2}\, e^{-\frac{1}{4}\sigma^2 r^2}, \tag{2.10}$$

Integrating the above ODE twice together with the condtion (2.9), we obtain

$$\varphi_1(\mathbf{x}) = -\frac{\widehat{\rho}(\mathbf{0})}{2}\, \left[\mathrm{E}_1(\sigma^2|\mathbf{x}|^2/4) + 2\ln(|\mathbf{x}|)\right], \tag{2.11}$$

where $\mathrm{E}_1(x) := \int_x^\infty t^{-1}e^{-t}\mathrm{d}t$ is the exponential integral function (see, for example, [1]).

REMARK 2.2. *φ_1 is not well defined at the origin in* (2.11)*. Instead, we should take the limit of $\mathbf{x}\to 0$ of the right hand side to obtain $\varphi_1(\mathbf{0})$. Straightforward computation shows that $\varphi_1(\mathbf{0}) = \widehat{\rho}(\mathbf{0})\left(\frac{\gamma}{2} + \ln\frac{\sigma}{2}\right)$, where $\gamma \approx 0.5772156649015328606$ is the Euler-Mascheroni constant.*

Second, we observe that the total charge in (2.8) is zero and thus the Fourier integral representation of the solution is well defined. That is,

$$\varphi_2(\mathbf{x}) = \frac{1}{2\pi}\int_{\mathbb{R}^2} \frac{\widehat{\rho}(\mathbf{k}) - \widehat{\rho}(\mathbf{0})\, e^{\frac{-|\mathbf{k}|^2}{\sigma^2}}}{|\mathbf{k}|^2}\, e^{i\,\mathbf{k}\cdot\mathbf{x}}\,\mathrm{d}\mathbf{k}. \tag{2.12}$$

Here we have used the fact that $\mathcal{F}(\rho(\mathbf{x}) - \widehat{\rho}(\mathbf{0})\frac{\sigma^2}{2}\, e^{-\frac{1}{4}\sigma^2|\mathbf{x}|^2}) = \widehat{\rho}(\mathbf{k}) - \widehat{\rho}(\mathbf{0})\, e^{\frac{-|\mathbf{k}|^2}{\sigma^2}}$. It is easy to see that $\widehat{\rho}(\mathbf{k}) - \widehat{\rho}(\mathbf{0})\, e^{\frac{-|\mathbf{k}|^2}{\sigma^2}}$ vanishes at the origin and the singularity at the origin in the definition of (2.12) can be removed by switching to polar coordinates. Thus, $\varphi_2(\mathbf{x})$ can be computed using the algorithms developed in [21].

REMARK 2.3. *The parameter σ in* (2.6) *should be chosen as large as possible under the constraint that the Gaussian $e^{-|\mathbf{k}|^2/\sigma^2}$ decays as fast as $\widehat{\rho}(\mathbf{k})$. This way,*

there is no need to enlarge the computational domain in the Fourier space. And secondly, there is no need to oversample the truncated Fourier domain due to the rapid decaying of the Gaussian. Thus, setting the Gaussian to $2\cdot 10^{-16}$ *at* $|\mathbf{k}|_\infty = L(B_k)/2\}$ *with* $L(B_k)$ *the sidelength of the computational box* B_k *in the Fourier space, we obtain* $\sigma = |\mathbf{k}|_\infty/6$.

We now summarize the algorithm of evaluating the Coulomb interaction in 2D as follows.

Algorithm 1 Evaluation of the Coulomb interaction in 2D

1: Evaluate $\varphi_1(\mathbf{x})$ via (2.11).
2: Evaluate $\varphi_2(\mathbf{x})$ using Algorithm 2 in [21].
3: Add φ_1 and φ_2 to obtain φ.

REMARK 2.4. *In many cases, one may need to solve the 2D free space Poisson equation multiple times on the same grid. Then one may compute* $E_1(\sigma^2|\mathbf{x}|^2/4) + 2\ln(|\mathbf{x}|)$ *only once on the grid and store them.*

3. A comparative study of the numerical methods of computing the ground state of the SPS. In this section, we first review the existing numerical methods (see, for example, [14,25,29] and references therein) for computing the ground state of the Schrödinger-Poisson system and modify them to incorporate our NUFFT-based algorithm for the potential evaluation. We then make a detailed comparative study about the accuracy and efficiency of our new method with other methods.

3.1. Computation of the ground state via NUFFT. For the Schrödinger-Poisson system (1.1), one quantity of great physical importance is the energy defined by the formula

$$E(\psi) := \int_{\mathbb{R}^d} \frac{1}{2}\,|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{1}{2}\,\beta\,\varphi|\psi|^2\,\mathrm{d}\mathbf{x}. \tag{3.1}$$

The ground state ϕ_g is defined as the minimizer of the energy E on the unit sphere $S = \{\phi\,|\|\phi\|_{L^2(\mathbb{R}^d)} = 1, E(\phi) < \infty\}$, i.e.,

$$\phi_g = \arg\,\min_{\phi\in S} E(\phi) \tag{3.2}$$

and the ground state energy is denoted as $E_g = E(\phi_g)$.

In order to compute the ground state of the SPS and the ground state energy, we use the method of *gradient flow* (GF) with discrete normalization [5,6,29]. The basic idea of the GF method is straightforward: instead of trying to solve the nonlinear eigenvalue problem directly, one tries to solve the associated time-dependent heat flow problem

$$\partial_t\phi(\mathbf{x},t) = -\frac{1}{2}\frac{\delta E(\phi)}{\delta\phi} = \left[\frac{1}{2}\Delta - V(\mathbf{x}) - \beta\varphi\right]\phi \tag{3.3}$$

with a properly chosen normalized initial state and march until a stable state is reached. The temporal direction is discretized into equispaced points $t_n = n\Delta t$ ($n = 0,1,2,\cdots$) and (3.3) is discretized via the backward Euler scheme

$$\frac{\phi(\mathbf{x},t_{n+1}^-) - \phi(\mathbf{x},t_n)}{\Delta t} = \left[\frac{1}{2}\Delta - V(\mathbf{x}) - \beta\varphi(\mathbf{x},t_n)\right]\phi(\mathbf{x},t_{n+1}^-). \tag{3.4}$$

Note here that the nonlinear term $\varphi(\mathbf{x}, t_n)$ is treated explicitly. After $\phi(\mathbf{x}, t_{n+1}^-)$ is obtain via an iterative Krylov solver (here a preconditioner developed in [2] is applied), the wave function is normalized again via the formula

$$\phi(\mathbf{x}, t_{n+1}) := \phi(\mathbf{x}, t_{n+1}^+) = \frac{\phi(\mathbf{x}, t_{n+1}^-)}{\|\phi(\mathbf{x}, t_{n+1}^-)\|} \tag{3.5}$$

so that it stays on the unit sphere. Due to the rapid decaying of the wave function, the spatial variable is truncated to a rectangular box and discretized into equispaced points. The action of the Laplacian operator is computed via the regular FFT. The action of the external potential V is computed via direct pointwise multiplication. And the nonlocal potential φ defined in (1.2) is evaluated via the algorithms presented in Section 2.

3.2. Comparisons of different numerical methods. In this section, we report numerical results on the computation of the ground state of the Schrödinger-Poisson system. For simplicity, the computational domain in space is truncated to a cubic box of length L; the number of discretization points in each spatial dimension is denoted by N; and the mesh size in each spatial dimension is denoted by $h = \frac{L}{N}$. We compare the performance of the following two methods: GF-NUFFT - the gradient flow method with potential evaluated via the NUFFT method, and GF-DST - the gradient flow method with potential evaluated via the DST method. We remark here that the standard FFT method for potential evaluation has even lower accuracy as compared with the DST method due to the "numerical locking" phenomenon discussed before. For both methods, the time marching is terminated when $\|\phi^{n+1} - \phi^n\|_{l^\infty} < \varepsilon$ with $\varepsilon = 10^{-12}$ for 2D problems and $\varepsilon = 10^{-10}$ for 3D problems, respectively. The numerical solution obtained with mesh size h is denoted by ϕ_g^h. And the errors shown here are in relative l^∞ norm.

EXAMPLE 3.1. *Ground state of the 2D SPS.* The external potential is chosen to be $V(x, y) = \frac{1}{2}(x^2 + 4y^2)$. The reference solution $\phi_g(\mathbf{x})$ is obtained numerically by *GF-NUFFT* with $\Delta t = 0.01$, $h = 1/16$, $\phi_0 = \pi^{-1/2} e^{-\frac{1}{2}(x^2+y^2)}$ on $[-16, 16]^2$. Table (3.1) lists the errors of the ground state and the Coulomb potential for $\beta = \pm 5$ on $[-8, 8]^2$.

Table 3.1: Errors of the ground state (upper) and the Coulomb potential (lower) for 2D SPS by *GF-NUFFT*.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$\beta = -5$	1.807E-02	7.507E-05	3.444E-10	2.109E-15
$\beta = 5$	7.273E-03	9.733E-06	5.982E-12	1.665E-15
$\beta = -5$	1.443E-02	2.948E-05	1.118E-10	2.451E-14
$\beta = 5$	3.989E-03	1.267E-06	1.036E-12	2.412E-14

EXAMPLE 3.2. *Ground state of the* $2.5D$ *SPS.* The external potential is the same as in Example (3.1) and the reference solution is computed by *GF-NUFFT* using the same parameters as in Example (3.1).

Table (3.2) lists the numerical results for the computation of the ground state by the GF-NUFFT method on $[-8, 8]^2$ with different mesh sizes. Table (3.3) lists the errors of the GF-DST method on the same computational domain $[-8, 8]^2$. Finally,

Table (3.4) lists the errors of the GF-DST method on $[-L, L]^2$ with the fine mesh size $h = 1/8$.

Table 3.2: Errors of the ground state (upper) and the Coulomb potential (lower) for 2.5D SPS by *GF-NUFFT* on $[-8, 8]^2$.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$\beta = -5$	3.619E-02	8.288E-04	4.364E-08	3.109E-15
$\beta = 5$	4.143E-03	1.393E-05	1.550E-10	1.221E-15
$\beta = -5$	3.968E-02	5.429E-04	3.192E-08	1.721E-15
$\beta = 5$	3.704E-03	9.501E-06	9.270E-11	4.996E-16

Table 3.3: Errors of the ground state for 2.5D SPS by *GF-DST* on $[-8, 8]^2$.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$	$h = 1/16$
$\beta = -5$	3.448E-02	1.562E-04	3.541E-05	3.541E-05	3.541E-05
$\beta = 5$	1.606E-03	3.613E-05	3.632E-05	3.632E-05	3.632E-05

Table 3.4: Errors of the ground state (upper) and the Coulomb potential (lower) for 2.5D SPS by *GF-DST* on $[-L, L]^2$ with $h = 1/8$.

	$L = 8$	$L = 16$	$L = 32$	$L = 64$
$\beta = -5$	3.541E-05	4.376E-06	5.455E-07	6.822E-08
$\beta = 5$	3.632E-05	4.460E-06	5.551E-07	6.931E-08
$\beta = -5$	1.995E-02	9.955E-03	4.150E-03	2.032E-03
$\beta = 5$	1.999E-02	9.960E-03	4.151E-03	2.032E-03

EXAMPLE 3.3. *Ground state of the 3D SPS.* The external potential is chosen to be radial symmetric: $V(x, y, z) = \frac{1}{2}(x^2 + y^2 + z^2)$. The reference solution is computed via the spectral method [14] on $r \in [0, 16]$ with $\Delta r = 1/16$ and a stricter stopping criterion $\|\phi^{n+1} - \phi^n\|_{l^\infty} < 10^{-12}$. We denote the reference solution by ϕ_g.

Table (3.5) presents the numerical results of the GF-NUFFT method and the GF-DST method with different mesh size for the coupling constant $\beta = \pm 5$. For both methods, the computational box in space is chosen to be $[-8, 8]^3$.

A comparison of Tables (3.2)-(3.4) shows that the GF-NUFFT method is spectrally accurate in space, while the errors of the GF-DST method are saturated at low accuracy, even though the enlargement of the computational domain may lower the saturation a bit.

EXAMPLE 3.4. *Virial identities.* When the external potential V is a homogeneous function of degree 2, i.e., $V(\lambda \mathbf{x}) = \lambda^2 V(\mathbf{x})$, then the stationary state $\phi_e(\mathbf{x})$ satisfies the following virial identities:

- for 2D SPS:

$$-2E_{\rm kin}(\phi_e) + 2E_{\rm pot}(\phi_e) - \frac{\beta}{4\pi} = 0,$$

Table 3.5: Errors of the ground states for the 3D SPS on $[-8,8]^3$ by *GF-NUFFT* (upper) and *GF-DST* (lower), respectively.

	$h=2$	$h=1$	$h=1/2$	$h=1/4$	$h=1/8$
			GF-NUFFT		
$\beta=-5$	5.362E-02	1.954E-04	2.201E-07	1.589E-11	8.232E-11
$\beta=\ 5$	6.098E-02	1.901E-04	1.624E-08	4.604E-11	4.843E-11
			GF-DST		
$\beta=-5$	1.034E-01	4.211E-03	7.300E-07	2.814E-07	2.814E-07
$\beta=\ 5$	6.693E-02	3.820E-04	3.351E-07	3.441E-07	3.441E-07

- for 2.5D and 3D SPS:

$$-2E_{\rm kin}(\phi_e)+2E_{\rm pot}(\phi_e)-E_{\rm int}(\phi_e)=0,$$

where $E_{\rm pot}(\phi_e)=\int_{\mathbb{R}^d}V(\mathbf{x})|\phi_e(\mathbf{x})|^2{\rm d}\mathbf{x}$, $E_{\rm int}(\phi_e)=\frac{\beta}{2}\int_{\mathbb{R}^d}\Phi(\mathbf{x})|\phi_e(\mathbf{x})|^2{\rm d}\mathbf{x}$ and $E_{\rm kin}(\phi_e)=\frac{1}{2}\int_{\mathbb{R}^d}|\nabla\phi_e|^2{\rm d}\mathbf{x}$. Obviously, the ground state ϕ_g is a stationary state. Thus the above identities also hold for ϕ_g.

We now check the accuracy of the ground state computation via the virial identities. We denote the numerical value of the left hand sides of the virial identities by $\mathcal{I}$. For two dimensional problems (i.e., 2D and 2.5D SPS), the external potential is chosen to be $V=\frac{1}{2}(x^2+4y^2)$. And for three dimensional, the external potential is chosen to be $V=\frac{1}{2}(x^2+y^2+4z^2)$. Both potentials are anisotropic. For all three cases, we set $h=1/8$ and the computational box to $[-8,8]^d$ $(d=2,3)$.

Tables (3.6) and (3.7) list the various energies associated with the ground state and the virial quantity $\mathcal{I}$ for 2D SPS, and 2.5D and 3D SPS with different coupling constant β.

Table 3.6: Energies of the ground state and virial identity difference for 2D SPS.

β	E_{kin}	E_{pot}	$\mathcal{I}$
-10	9.8061E-01	5.8272E-01	2.4514E-08
-5	8.5784E-01	6.5889E-01	2.5560E-08
-1	7.7024E-01	7.3045E-01	2.6013E-08
1	7.3046E-01	7.7025E-01	-2.6341E-08
5	6.5959E-01	8.5854E-01	-2.7257E-08
10	5.8770E-01	9.8559E-01	-2.8184E-08

4. A comparative study of the numerical methods of computing the dynamics of the SPS. In this section, we first incorporate our NUFFT algorithm for the potential evaluation into the well-known time-splitting method to obtain a new method for computing the dynamics of the SPS. We then present a detailed comparative study about the accuracy and efficiency of our new method with the method using the DST for potential evaluation.

4.1. Computation of the dynamics via NUFFT. In order to solve the time-dependent Schrödinger-Poisson equation (1.1), we first note that the following time evolution operator is exact:

$$\psi(\mathbf{x},t_{n+1})=e^{-i[-\frac{1}{2}\Delta+V(\mathbf{x})+\beta\varphi(\mathbf{x},t_n)](t_{n+1}-t_n)}\psi(\mathbf{x},t_n). \tag{4.1}$$

Table 3.7: Energies of the ground state and virial identity difference for 2.5D and 3D SPS.

β	E_{kin}	E_{pot}	E_{int}	$\mathcal{I}$
		2.5D SPS		
-10	1.2611E00	4.6592E-01	-1.5903E00	1.8530E-08
-5	9.4226E-01	6.0401E-01	-6.7651E-01	2.3424E-08
-1	7.8098E-01	7.2058E-01	-1.2080E-01	2.5971E-08
1	7.2201E-01	7.7942E-01	1.1483E-01	-2.6384E-08
5	6.3379E-01	8.9629E-01	5.2501E-01	-2.6559E-08
10	5.5977E-01	1.0385E00	9.5748E-01	-2.7310E-08
		3D SPS		
-10	1.0990E00	9.1197E-01	-3.7401E-01	-3.5086E-06
-5	1.0467E00	9.5594E-01	-1.8147E-01	-3.7927E-06
-1	1.0089E00	9.9118E-01	-3.5462E-02	-3.9957E-06
1	9.9128E-01	1.0088E00	3.5064E-02	-4.1400E-06
5	9.5831E-01	1.0441E00	1.7151E-01	-4.3640E-06
10	9.2101E-01	1.0880E00	3.3408E-01	-4.7469E-06

It is clear that the kinetic energy part, i.e., the Laplacian operator does not commute with the potential operator. However, the well-known splitting method splits the kinetic operator and the potential operator and computes their actions separately. For example, the second-order Strang splitting [27] splits the time evoluation operator as follows:

$$\begin{aligned}\psi(\mathbf{x}, t_{n+1}) = & e^{-\frac{i}{2}[V(\mathbf{x})+\beta\varphi(\mathbf{x},t_n)](t_{n+1}-t_n)} \\ & \cdot e^{\frac{i}{2}\Delta(t_{n+1}-t_n)} \cdot e^{-\frac{i}{2}[V(\mathbf{x})+\beta\varphi(\mathbf{x},t_n)](t_{n+1}-t_n)}\psi(\mathbf{x}, t_n).\end{aligned} \tag{4.2}$$

The order of accuracy can be increased by performing this symmetric splitting more times, and we have actually implemented a fourth order splitting scheme in our code. We truncate the spatial domain to a rectangular box and discretize the spatial variable into equispace points in the box. The action of the potential operator is carried out via pointwise multiplication. And the action of the Laplacian operator is carried out in the Fourier space via FFT. Finally, the evaluation of the Coulomb interaction were carried out via either the standard FFT or the DST methods. We now use our NUFFT based algorithm instead to evaluate the Coulomb interaction φ.

4.2. Comparisons of different numerical methods. We report here the numerical results for the computation of the synamics of the Schröding-Poisson system. We compare two methods: TS-NUFFT - the fourth-order time splitting Fourier pseudospectral method with the Coulomb interaction evaluated by the NUFFT algorithm; and TS-DST - the fourth-order time splitting Fourier pseudospectral method with the Coulomb interaction evaluated by the DST algorithm. All the errors reported here are in relative l^2 norm.

EXAMPLE 4.1. *Dynamics of the 2D SPS.* We compute the wavefunction $\psi(\mathbf{x}, t)$ and the nonlocal potential φ at time $T = 1/2$ by *TS-NUFFT* under the external potential $V(x, y) = \frac{1}{2}\ (x^2 + y^2)$, with the initial value $\psi(\mathbf{x}, 0) = e^{-\frac{1}{2}(x^2+y^2)}$. The reference wavefunction and the potential are obtained by *TS-NUFFT* with $\Delta t = 0.0001$ and $h = 1/16$ on $[-16, 16]^2$.

Table (4.1) lists errors of the wavefunction and the Coulomb potential obtained by *TS-NUFFT* with different mesh size h for $\beta = \pm 5$.

Table 4.1: Errors of the wavefunction (top) and the Coulomb potential (bottom) for 2D SPS by *TS-NUFFT*.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$\beta = -5$	7.830E-02	2.309E-04	2.489E-09	1.847E-12
$\beta = 5$	3.207E-02	9.381E-05	8.459E-12	2.476E-12
$\beta = -5$	1.819E-02	7.112E-05	7.910E-10	5.660E-12
$\beta = 5$	6.763E-03	2.932E-06	1.173E-11	8.318E-12

EXAMPLE 4.2. *Dynamics of the* 2.5*D SPS.* We compute the wavefunction $\psi(\mathbf{x}, t)$ and the nonlocal potential $\varphi(\mathbf{x}, t)$ at time $T = 1/2$ by *TS-NUFFT* under the external potential $V(x, y) = \frac{1}{2}(x^2 + y^2)$ with the initial value $\psi(\mathbf{x}, 0) = e^{-\frac{1}{2}(x^2+y^2)}$. The reference wavefunction and the potential are obtained by *TS-NUFFT* with $\Delta t = 0.0001$ and $h = 1/16$ on $[-16, 16]^2$.

Table 4.2 lists errors of the wavefunction and the Coulomb potential on $[-8, 8]^2$ with different mesh size h by the TS-NUFFT method. Table 4.3 lists errors of the wavefunction and the Coulomb potential on $[-16, 16]^2$ with different mesh size h by the TS-DST method. And Table 4.4 lists errors of the wavefunction and the Coulomb potential on $[-L, L]^2$ with $h = 1/8$ by the TS-DST method.

Table 4.2: Errors of the wavefunction (top) and the COulomb potential (bottom) for 2.5D SPS by *TS-NUFFT*.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$\beta = -5$	9.801E-04	1.052E-04	1.853E-07	6.568E-13
$\beta = 5$	6.450E-02	7.108E-04	7.171E-10	2.413E-12
$\beta = -5$	3.280E-02	2.965E-03	2.129E-06	1.866E-12
$\beta = 5$	2.340E-02	1.553E-04	3.942E-11	1.359E-12

Table 4.3: Errors of the wavefunction (top) and the Coulomb potential (bottom) for 2.5D SPS by *TS-DST* on $[-16, 16]^2$.

	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$\beta = -5$	2.1936E-01	1.1083E-01	1.1191E-01	1.1191E-01
$\beta = 5$	1.3120E-01	1.1194E-01	1.1194E-01	1.1194E-01
$\beta = -5$	8.5466E-01	8.5212E-01	8.5207E-01	8.5207E-01
$\beta = 5$	8.2375E-01	8.3799E-01	8.4521E-01	8.4881E-01

EXAMPLE 4.3. *Dynamics of the 3D SPS.* Consider the dynamics of 3D SPS at time $T = 1/8$ with initial wavefunction $\psi_0(x, y, z) = e^{-\frac{x^2+y^2+z^2}{2}}$ under the external potential $V = \frac{1}{2}(x^2 + y^2 + z^2)$. The reference solution is obtained by the TS-NUFFT method with $\Delta t = 0.001$ and $N = 256$.

Table 4.4: Errors of the wavefunction (top) and the Coulomb potential (bottom) for 2.5D SPS by *TS-DST* on $[-L, L]^2$ with $h = 1/8$.

	$L = 8$	$L = 16$	$L = 32$	$L = 64$
$\beta = -5$	2.2413E-01	1.1191E-01	5.5934E-02	2.7964E-02
$\beta = 5$	2.2441E-01	1.1194E-01	5.5938E-02	2.7965E-02
$\beta = -5$	8.5307E-01	8.5207E-01	4.1045E-01	2.0280E-01
$\beta = 5$	8.5452E-01	8.5242E-01	4.1048E-01	2.0280E-01

Table 4.5 lists errors of the wavefunction and the Coulomb potential of the 3D SPS by *TS-NUFFT* with different mesh size h for $\beta = \pm 5$.

Table 4.5: Errors of the wavefunction (top) and the Coulomb potential (bottom) for 3D SPS by *TS-NUFFT*.

	$h = 2$	$h = 1$	$h = 1/2$	$h = 1/4$	$h = 1/8$
$\beta = -5$	3.749E-01	6.102E-03	1.533E-05	2.028E-11	3.988E-12
$\beta = 5$	2.008E-01	4.450E-03	1.430E-05	1.877E-11	4.181E-12
$\beta = -5$	1.453	5.164E-03	3.283E-06	9.356E-12	4.910E-12
$\beta = 5$	1.453	4.411E-03	2.176E-06	7.721E-12	4.921E-12

From Tables 4.2 and 4.5, we observe that the *TS-DST* method can not resolve the wavefunction or the potential very accurately while the TS-NUFFT method achieves the spectral accuracy in space for both the wavefunction and the potential.

5. Conclusion. We have extend the algorithm in [21] to evaluate the Coulomb interactions in two dimensions. The algorithm is based on NUFFT and has $O(N \log N)$ complexity with a small prefactor. The algorithm is spectrally accurate for smooth densities and applicable even when the potential grows logarithmically at infinity.

We have also incorporated our NUFFT-based algorithm for the potential evaluation into the popular schemes for computing the ground state and dynamics of the Schrödinger-Poisson system. A detailed and systematic comparison has been carried out to demonstrate the advantages of our new method. The numerical experiments show that our new method only requires a computational box large enough to hold the (numerical) support of the wave function and needs much fewer points inside the box to achieve higher order of accuracy as compared with the existing methods using the standard FFT or the DST.

We are currently incorporating our new algorithm into the solver for computing the ground state and dynamics of the dipole-dipole interaction of Bose-Einstein condensates. The results will be reported on a later date.

Acknowledgments. Part of this work was done when the authors were visiting Beijing Computational Science Research Center in the summer of 2014.

REFERENCES

[1] M. Abbamowitz and I. A. Stegun, *Handbook of Mathematical Functions*, Dover, 1965.

[2] Xavier Antoine, Romain Duboscq, *Robust and efficient preconditioned Krylov spectral solvers for computing the ground states of fast rotating and strongly interacting Bose-Einstein condensates*, J. Comput. Phys., 258 (2014), pp. 509–523.

[3] W. Bao and Y. Cai, *Mathematical theory and numerical methods for Bose-Einstein condensation*, Kinet. Relat. Mod., 6 (2013), pp. 1–135.

[4] W. Bao, Y. Cai and H. Wang, *Efficient numerical methods for computing ground states and dynamics of dipolar Bose-Einstein condensates*, J. Comput. Phys., 229 (2010), pp. 7874–7892.

[5] W. Bao, I-L. Chern and F. Y. Lim, *Efficient and spectrally accurate numerical methods for computing ground and first excited states in Bose-Einstein condensates*, J. Comput. Phys., 219 (2006), pp. 836–854.

[6] W. Bao and Q. Du, *Computing the ground state solution of Bose-Einstein condensates by a normalized gradient flow*, SIAM J. Sci. Comput., 25 (2004), pp. 1674–1697.

[7] W. Bao, H. Jian, N.J. Mauser and Y. Zhang,*Dimension reduction of the Schrödinger equation with Coulomb and anisotropic confining potentials*, SIAM J. Appl. Math., 73 (6) (2013), pp. 2100–2123.

[8] W.Z. Bao, P.A. Markowich, Q.L. Tang and Y. Zhang, *Robust and efficient numerical methods for computing ground state and dynamics of dipolar Bose-Einstein condensation*, preprint.

[9] W. Bao, D. Marahrens, Q. Tang and Y. Zhang, *A simple and efficient numerical method for computing the dynamics of rotating Bose-Einstein condensates via a rotating Lagrangian coordinate*, SIAM J. Sci. Comput., 35 (6) (2013), pp. A2671–A2695.

[10] W. Bao, N. J. Mauser and H. P. Stimming, *Effective one particle quantum dynamics of electrons: A numerical study of the Schrödinger-Poisson-Xα model*, Comm. Math. Sci., 1 (2003), pp. 809–831.

[11] N. Ben Abdallah, F. Méhats and O. Pinaud, *Adiabatic approximation of the Schrödinger-Poisson system with a partial confinement*, SIAM J. Math. Anal., 36 (2005), pp. 986–1013.

[12] Y. Cai, M. Rosenkranz, Z. Lei and W. Bao, *Mean-field regime of trapped dipolar Bose-Einstein condensates in one and two dimensions*, Phys. Rev. A, 82 (2010), 043623.

[13] T. Cazenave, *Semilinear Schrödinger equations*, Courant Lecture Notes in Mathematics, vol. 10, New York University Courant Institute of Mathematical Sciences AMS, 2003.

[14] X. Dong, *A short note on simplified pseudospectral methods for computing ground state and dynamics of spherically symmetric Schrödinger-Poisson-Slater system*, J. Comput. Phys., 230 (2011), pp. 7917–7922.

[15] A. Dutt and V. Rokhlin, *Fast Fourier transforms for nonequispaced data*, SIAM J. Sci. Comput., 14 (1993), pp. 1368–1393.

[16] F. Ethridge and L. Greengard, *A new fast-multipole accelerated Poisson solver in two dimensions*, SIAM J. Sci. Comput., 23 (3) (2001), pp. 741–760.

[17] L. Genovese, T. Deutsch, A. Neelov, S. Goedecker and G. Beylkin, *Efficient solution of Poisson equation with free boundary conditions*, J. Comput. Chem., 125 074105 (2006).

[18] Z. Gimbutas, L. Greengard and M. Minion, *Coulomb interactions on planar structures: inverting the square root of the Laplacian*, SIAM J. Sci.Comput., 22 (6) (2000), pp. 2093–2108.

[19] L. Greengard and J.Y. Lee, *Accelerating the nonuniform fast Fourier transform*, SIAM Rev., 46 (2004), pp. 443–454.

[20] L. Greengard and V. Rokhlin,*A new version of the fast multipole method for the Laplace equation in three dimensions*, Acta Numerica, 6 (1997), pp. 229–269.

[21] S. Jiang, L. Greengard and W. Bao, *Fast and Accurate Evaluation of Nonlocal Coulomb and Dipole-Dipole Interactions via the Nonuniform FFT*, SIAM J. Sci. Comput., accepted.

[22] S. Jin, H. Wu and X. Yang, *A numerical study of the Gaussian beam methods for one-dimensional Schrödinger-Poisson equations*, J. Comput. Math, 28 (2010), pp. 261–272.

[23] S. Masaki, *Energy solution to a Schrödinger-Poisson system in the two-dimensional whole space*, SIAM J. Math. Anal., 43 (2011), pp. 2719–2731.

[24] F. Méhats, *Analysis of a quantum subband model for the transport of partially confined charged particles*, Monatch. Math., 147 (2006), pp. 43–73.

[25] N.J. Norbert and Y. Zhang, *Exact artificial boundary condition for the Poisson equation in the simulation of the 2D Schrödinger-Poisson system*, Commun. Comput. Phys., to appear.

[26] H.P. Stimming and Y. Zhang, *Efficient and accurate computation of the Davey-Stewartson equation via nonuniform FFT*, submitted.

[27] G. Strang, *On the construction and comparision of difference schemes*, SIAM J. Numer. Anal., 5 (1968),pp. 505-517.

[28] H. Yoshida, *Construction of higher order symplectic integrators*, Phys. Lett. A., 150 (1990), pp. 262–268.
[29] Y. Zhang and X. Dong, *On the computation of ground states and dynamics of Schrödinger-Poisson-Slater system*, J. Comput. Phys., 230 (2011), pp. 2660–2676.