Journal of Magnetism and Magnetic Materials 400 (2016) 99–102

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Influence of variations in the electron–electron interaction on the ground state metric space "band structure" of a two-electron magnetic system

P.M. Sharp *, I. D'Amico

Department of Physics and York Centre for Quantum Technologies, University of York, York, YO10 5DD, United Kingdom

ARTICLE INFO

Article history:
Received 20 June 2015
Received in revised form
12 August 2015
Accepted 14 August 2015
Available online 17 August 2015

Keywords:
Metric spaces
Current Density Functional Theory
Systems in magnetic fields

ABSTRACT

We consider a model system of two electrons confined in a two-dimensional harmonic oscillator potential, with the electrons interacting via an α/r^2 potential, and subject to a magnetic field applied perpendicular to the plane of confinement. Our results show that variations in the strength of the electron–electron interaction generate a "band structure" in ground state metric spaces, which shares many characteristics with those generated as a result of varying the confinement potential. In particular, the metric spaces for wavefunctions, particle densities, and paramagnetic current densities all exhibit distinct "bands" and "gaps". The behavior of the polar angle of the bands also shares traits with that obtained by varying the confinement potential, but the behavior of the arc lengths of the bands on the metric space spheres can be seen to be different for the two cases and opposite for a large range of angular momentum values. The findings here and in Refs. [1,2] demonstrate that the "band structure" that arises in ground state metric spaces when a magnetic field is applied is a robust feature.

1. Introduction

The metric space approach to quantum mechanics [1,3] is a new method to study the properties of quantum mechanical functions by the analysis of the behavior of related metrics derived from physical conservation laws. This approach has so far been used on systems with [1,2] and without [3,4] applied magnetic fields, and has provided new insights into Density Functional Theory [3] and Current Density Functional Theory (CDFT) [1,2]. CDFT [5,6] is used to describe interacting systems subject to magnetic fields, and the fundamental mapping at its core states that, for ground states, the wavefunction is uniquely determined by the particle density together with the paramagnetic current density and vice versa. While this mapping is formally well defined, its characteristics are unknown, and furthering its understanding is crucial to improve the ability of CDFT-based procedures to predict the properties of systems in magnetic fields.

When analyzing this mapping with the metric space approach, and for the systems studied, it was found that the ground states' metric spaces, for all the physical functions involved in the mapping, displayed a distinctive "band structure": when varying the confinement potential [1] the "band structure" consists of allowed ("bands") and forbidden ("gaps") distances, with points grouped into bands according to the value of the magnetic quantum number, m [1]. When varying instead the magnetic field [2], it was observed that for wavefunctions and particle densities, this "band structure" consisted of "overlapping bands", with the "bands and gaps" structure persisting for the paramagnetic current density.

In this paper we will further examine this "band structure" by considering the effect of varying the strength of the interaction between the electrons.

2. Metrics

In order to study the core mapping of CDFT, we require metrics for wavefunctions, particle densities and paramagnetic current densities. Taking conservation laws for the wavefunction norm, particle number and z-component of angular momentum, and following the metric space approach to quantum mechanics, we introduce the following metrics:

* Corresponding author.
E-mail addresses: pms510@york.ac.uk (P.M. Sharp), irene.damico@york.ac.uk (I. D'Amico).

http://dx.doi.org/10.1016/j.jmmm.2015.08.061
0304-8853/

$$D_\psi(\psi_1, \psi_2) = \left[\int \left(|\psi_1|^2 + |\psi_2|^2 \right) d\mathbf{r}_1 \ldots d\mathbf{r}_N - 2 \left| \int \psi_1^* \psi_2 d\mathbf{r}_1 \ldots d\mathbf{r}_N \right| \right]^{1/2}, \quad (1)$$

$$D_\rho(\rho_1, \rho_2) = \int \left| \rho_1(\mathbf{r}) - \rho_2(\mathbf{r}) \right| d\mathbf{r}, \quad (2)$$

$$D_{\mathbf{j}_{p_\perp}}(\mathbf{j}_{p_1}, \mathbf{j}_{p_2}) = \int \left| \left\{ \mathbf{r} \times \left[\mathbf{j}_{p_1}(\mathbf{r}) - \mathbf{j}_{p_2}(\mathbf{r}) \right] \right\}_z \right| d\mathbf{r}, \quad (3)$$

for wavefunctions ψ, particle densities ρ, and paramagnetic current densities $\mathbf{j}_p$ respectively [1,3]. Each of these metrics has an "onion-shell" geometry that consists of concentric spheres [1–3] of radius $\sqrt{N}$, N, and m respectively, with N being the number of particles.

3. Model system

We will apply our metrics to a model system which consists of two electrons confined in a two-dimensional harmonic oscillator potential, with the electrons interacting via an α/r^2 potential, and subject to a magnetic field $\mathbf{B} = \omega_c c\hat{z}$ applied perpendicular to the plane of confinement [7]. This system has the significant advantage that the Schrödinger equation is now exactly solvable for arbitrarily strong confinement potentials, many-body interactions, and magnetic fields. The Hamiltonian for this system is [7]

$$\hat{H} = \sum_{i=1}^{2} \left[\frac{1}{2} \left(\mathbf{p}_i + \frac{1}{c} \mathbf{A}(\mathbf{r}_i) \right)^2 + \frac{1}{2} \omega_0^2 r_i^2 \right] + \frac{\alpha}{(\mathbf{r}_2 - \mathbf{r}_1)^2}, \quad (4)$$

where, in the symmetric gauge, $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{B} \times \mathbf{r}$. By solving the Schrödinger equation, we can generate wavefunctions, particle densities, and paramagnetic current densities for any value of α, the parameter controlling the strength of the interaction between the two electrons.

We generate a family of ground states by varying α, while holding the confinement frequency, ω_0, cyclotron frequency ω_c, and all other parameters in the Hamiltonian constant. As was the case in Refs. [1,2], we must change the value of the quantum number m as we change α in order to ensure that we remain in the ground state, which is essential for the core mapping of CDFT to hold.

We choose the value $\alpha = 29.756$ as a reference, and then each metric is used to find the distance between the related function at the reference and all of the other elements of the family. This value of α is chosen such that most of the available distance range is explored for both increasing and decreasing α, and that the reference state lies exactly halfway within the range of values of α for $m = -15$.

4. Effect of varying the electron interaction on metric space "band structures"

Fig. 1 shows plots of all of the distances with respect to one another as the parameter α is varied. In the plots the distance $D_{\mathbf{j}_{p_\perp}}$ is rescaled as $(2/|m_1| + |m_2|)D_{\mathbf{j}_{p_\perp}}$. All of the plots show a "band structure" which depends on the changes in the value of the angular momentum quantum number m, consisting of "bands" of distances for each particular value of m separated by "gaps" of forbidden distances. This is similar to what was found when considering variations of the external confinement potential [1]. When considering D_ρ against D_ψ [Fig. 1(a)], the path traced out by the curve is almost identical to that in Fig. 2 in Ref. [1], and again depicts a monotonic relationship between D_ρ and D_ψ which is almost linear for small to intermediate distances and follows the same curve for the cases of increasing α and decreasing α. Fig. 1 (b) and 1(c) shows that the "band structure" causes discontinuities in the gradient of the curves when we introduce the paramagnetic current density. However, in contrast to Ref. [1], the discontinuity in the gradient between "bands" is considerably less pronounced, and also as $|m|$ decreases, the bands cover a smaller range of distances. Comparison of the results in Ref. [1] and Fig. 1 suggests that as the reference value of $|m|$ becomes larger, the discontinuity in

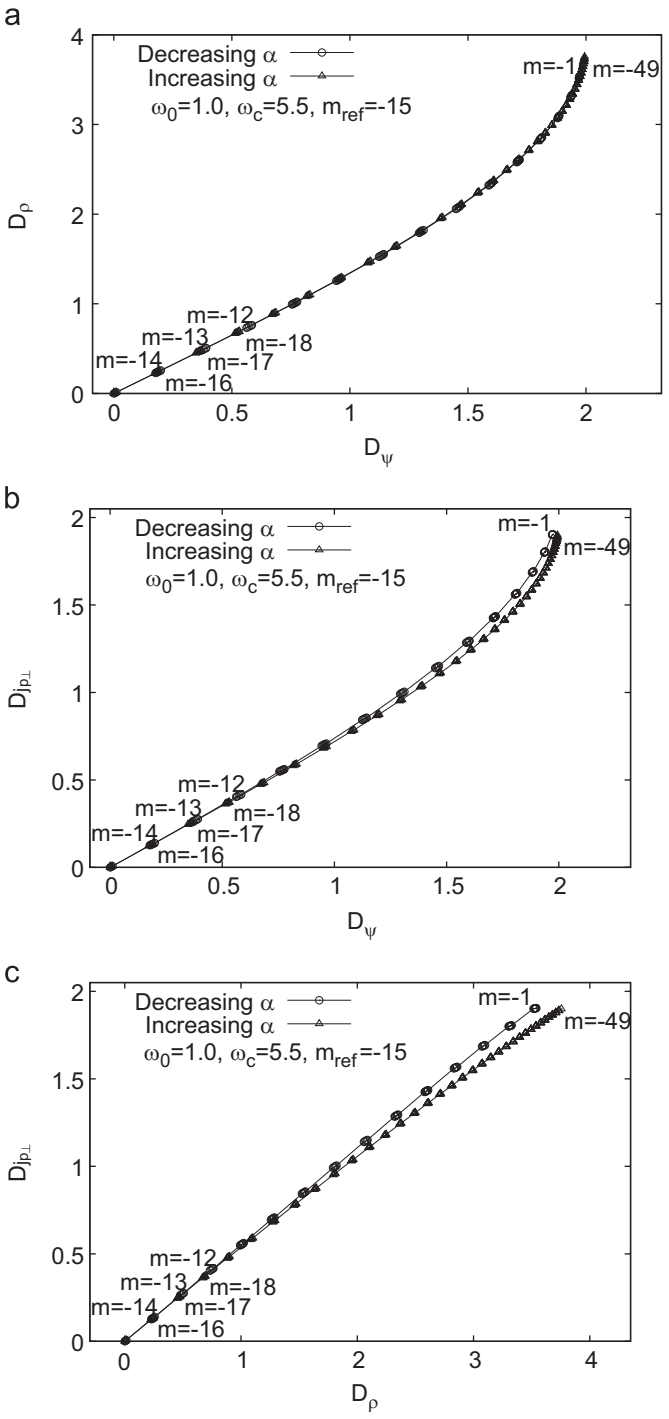

Fig. 1. Results for ground states when varying alpha (reference state $\omega_0 = 1.0$, $\omega_c = 5.5$, $\alpha = 29.756$, and $m_{ref} = -15$). The reference value of α is taken halfway between the range of values related to m_{ref}. Panel (a): D_ρ vs D_ψ; (b): rescaled $D_{\mathbf{j}_{p_\perp}}$ vs D_ψ; (c): rescaled $D_{\mathbf{j}_{p_\perp}}$ vs D_ρ. Values of alpha smaller than the reference are labeled with circles, larger with triangles.