Generalized Scaling Law for Exciton Binding Energy in Two-Dimensional Materials

S. Ahmad, M. Zubair, O. Jalil, M. Q. Mehmood, U. Younis, X. Liu, K. W. Ang, and L. K. Ang

1 Electrical Engineering Department, Information Technology University (ITU) of the Punjab, Lahore 54000, Pakistan
2 NanoTech Lab, Electrical Engineering Department, Information Technology University (ITU) of the Punjab, Lahore 54000, Pakistan
3 College of Materials Science and Engineering, Shenzhen Key Laboratory of Microscale Optical Information Technology, Chinese Engineering and Research Institute of Microelectronics, Shenzhen University, 3688 Nanhai Avenue, Shenzhen 518060, People’s Republic of China
4 Department of Electrical and Computer Engineering, National University of Singapore, 4 Engineering Drive 3, Singapore 117583, Singapore
5 Science and Math Cluster, Singapore University of Technology and Design (SUTD), 8 Somapah Road, Singapore 487372, Singapore

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Binding energy calculation in two-dimensional (2D) materials is crucial in determining their electronic and optical properties pertaining to enhanced Coulomb interactions between charge carriers due to quantum confinement and reduced dielectric screening. Based on full solutions of the Schrödinger equation in a screened hydrogen model with a modified Coulomb potential \(1/r^\beta\), we present a generalized and analytical scaling law for the exciton binding energy, \(E_\beta = E_0 (a\beta^b + c) (\mu/\epsilon)^w\), where \(\beta\) is a fractional-dimension parameter that accounts for the reduced dielectric screening. The model is able to provide accurate binding energies, benchmarked using the reported Bethe-Salpeter equation and experimental data, for 58 monolayer 2D and eight bulk materials, respectively, through \(\beta\). For a given material, \(\beta\) is varied from \(\beta = 3\) for bulk three-dimensional materials to a value lying in the range 2.55–2.7 for 2D monolayer materials. With \(\beta_{\text{mean}} = 2.625\), our model improves the average relative mean square error by a factor of 3 in comparison to existing models. The results can be used for Coulomb engineering of exciton binding energies in the optimal design of 2D materials.

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I. INTRODUCTION

Accurate determination of optical and electronic properties of bulk and two-dimensional (2D) materials is crucial for many applications, especially when the excitonic effects become significant in the 2D regime due to structural changes induced by dielectric environments leading to variation in binding energies [1–10]. The 2D nature of the material makes the excitons easily tunable, with some external stimuli, enabling excitonic-transport-based photonic devices such as electrically driven light emitters, optovalletronic devices, photovoltaic solar cells, and lasers [11–13]. Thus the binding-energy calculation in 2D materials has become an active area of research and numerous studies based on theoretical and experimental approaches have been reported in the literature to understand the excitonic effects and their implications [14–18]. Due to the high cost of experimental procedures, reliance on numerical approaches such as the Bethe-Salpeter equation (BSE) becomes inevitable for accurate modeling of excitonic effects and thus serves as a benchmark for other models [19]. In order to reduce the computational complexity, analytical methods are desirable to speed up the design processes [20–22]. A number of models to describe exciton behavior have been reported, including the pioneering works of Frenkel and Wannier-Mott (W-M) [23,24]. The Frenkel model is based on the concept of localized screening, whereas the W-M model incorporates an average delocalized screening effect irrespective of the actual dielectric environment and thus leads to an overestimation of binding energies. Olsen et al. [25] introduced an effective dielectric screening based on material polarizability, resulting in relatively accurate binding...
energies. Recently, a generalized extension of the model by Jiang et al. [26] has found the 2D exciton binding energy to be one fourth of the band gap, resulting in error reduction. The difficulty with the existing models is that the inherent Coulomb screening potential does not take the structural-confinement effects into account and therefore the accuracy in 2D binding-energy calculations is compromised. Therefore, we propose a simple approach to explicitly incorporate the structural-confinement effects in the screening potential by representing the Coulomb potential in a fractional space to represent a more realistic dielectric environment in an effective manner. Moreover, the realistic systems are not 2D in a strict sense and the fields, including the electric field and the magnetic field, the electron emission, and the angular momentum, are not confined to a smooth plane [27]. Hence, the central force between the electron and the nucleus may be better represented by a generalized Coulomb potential function, assuming that the system lies in an equivalent fractional-dimensional space. It is worthwhile to mention that the concept of fractional-dimensional space has been successfully applied to study the effects of confinement, roughness, and disorder in various physical problems arising in electron-device modeling [28,29], plasma physics [30], and electromagnetism [31].

Motivated by the above, the purpose of this paper is to develop an analytical scaling law for the binding-energy mean square errors (MSEs) of 39.2% and 26%, respectively, whereas the proposed FCP model (at $\beta_{\text{mean}} = 2.625$) reduces the average MSE to below 12.8%.

Finally, we show that there exists a simple scaling with a smooth transition of $\beta$ corresponding to structural confinement from bulk to the monolayer regime.

II. FORMULATION

The FCP model is based on a fractional Coulomb potential embedded in an infinite quantum well given by the radial part of a simple hydrogen model as

$$\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_{\text{frac}}(r) \right] \psi(r) = E\psi(r),$$

(1)

where $\mu = 0.9995m_0$ ($m_0 = 9.11 \times 10^{-31}$ kg) is the exciton reduced mass, $r$ is the radial distance, and $V_{\text{frac}}(r)$ is the fractional Coulomb potential. The fractional Coulomb potential is a generalized form of the standard Coulomb potential that exhibits a Coulomb-like electron-hole pair interaction and is based on the fractional-dimensional Poisson equation [31–33] of the form

$$\nabla^2_\beta V_{\text{frac}}(r) = -\rho/\epsilon,$$

(2)

where $\beta$ is a fractional-dimension parameter that is valid in the range $2 < \beta \leq 3$, $\rho$ is the volume charge density, and $\nabla^2_\beta$ is a generalized fractional-dimensional Laplacian operator in spherical coordinates [34], with the radial component given by

$$\nabla^2_\beta = \frac{1}{r^{\beta-1}} \frac{\partial}{\partial r} \left[ r^{\beta-1} \frac{\partial}{\partial r} \right].$$

(3)

Following the analytical solution of Eq. (2) from Ref. [32], the fractional Coulomb potential takes the form

$$V_{\text{frac}}(r) = k_\beta e^2/r^{\beta-2},$$

(4)

where $k_\beta = \Gamma(\beta/2)/[2\pi^{\beta/2}(\beta - 2)e_0]$. At $\beta = 3$, $k_\beta$ reduces to $1/4\pi\epsilon_0$ and $V_{\text{frac}}(r)$ simplifies to the standard Coulomb potential of the form $1/r$. When $\beta$ differs from three, the Coulomb potential of a point source falls off as $1/r^{\beta-2}$ and the dynamical symmetry is broken; this is effectively linked to the reduced hydrogenic screening and leads to an effective reduction in the Bohr radius.

The full solution to Eq. (1) is performed (for the detailed derivation, see the Appendix) to calculate the ground-state hydrogenic energy $e_\beta(\beta)$, where $e_\beta(\beta) = E_0(\beta)/13.6$ eV. A power-law fit to the full solution of Eq. (1) is performed to develop an analytical scaling law for the binding-energy
calculation, given by

\[ E_\beta = E_0(a\beta^b + c) \left( \frac{\mu}{\epsilon^2} \right), \]  

(5)

where \( E_0 = 13.6 \text{ eV}, \) \( a\beta^b + c \approx e_0(\beta), \) \( a = -2.619 \times 10^4, \) and \( b = -9.634 \) and \( c = -0.3833 \) are the fitting parameters obtained from a power-law fit to \( e_0(\beta) \) with 95% confidence intervals of \((-2.867 \times 10^4, -2.37 \times 10^4), \) \((-9.749, -9.519), \) and \((-0.4164, -0.3502), \) respectively. Here, \( \epsilon \) is the dielectric constant, calculated using \( \frac{1}{2}(1 + \sqrt{1 + 32\pi a\mu/3}), \) which represents the effective linear screening for the strict 2D case [25]. \( \mu \) is the reduced exciton mass, and \( a \) is the 2D polarizability based on reported data for \( G_0 W_0 \) [19].

An infinite quantum-well (QW) equivalence of the FCP model in Eq. (1) is demonstrated to explain an effective reduction in the Bohr radius. The fractional Coulomb potential for \( 2.5 \leq \beta \leq 3 \) is calculated using Eq. (4) and is plotted against a radial distance \( r \) corresponding to \( \beta = 3, \) as illustrated in Fig. 2. A radial distance of approximately 20 times the Bohr radius (19.75 \( a_0 \), where \( a_0 = 0.529 \text{Å} \)) with a uniform mesh grid of 300 points is taken to emulate the full-wave behavior of the FCP model, which is necessary for convergence (for details, see the Appendix). Here, the radial distance is equivalent to an infinite QW width and is highlighted to shrink with decreasing values of \( \beta. \) This is validated by first computing the ground-state hydrogenic energies \( E_0(\beta) \) for \( 2.5 \leq \beta \leq 3 \) using the FCP model in Eq. (1), as shown in the inset of Fig. 2. The resulting values of \( E_0(\beta) \) are then employed to calculate the corresponding infinite QW width \( w, \) using

\[ w = \sqrt{\hbar^2 \pi^2 / 2\mu E_0(\beta)}, \]  

(6)

which is in excellent agreement with the radial distance \( r \) as shown in Fig. 3. The decrease in \( w \) corresponds to a reduction in the effective Bohr radius given by \( a_\beta = w / 19.75, \) as illustrated in the inset of Fig. 3. The reduction in \( a_\beta \) takes place due to a proportionate decrease in the QW dimensions, as a well width of at least 19.75 \( a_\beta \) is required for the infinite QW model to produce hydrogenic energies \( E_0(\beta). \)
III. RESULTS AND DISCUSSION

The significance of the fractional Coulomb potential in the 2D binding-energy calculation is highlighted by performing a comparison of the existing analytical methods with the proposed FCP model by using BSE-reported binding energies for 58 monolayers as a benchmark [19]. The analysis is performed to intercept \( \beta \) based on the FCP model in Eq. (5) for binding energies reported using the BSE and that calculated using existing analytical models. The result in Fig. 4 shows that the FCP model accurately produces results through \( \beta \), with most of the monolayer materials found to lie at \( \beta \) values in the range 2.55–2.7, to represent the actual 2D exciton screening, whereas the W-M model is shown to overestimate the 2D binding energies, with the average screening represented by a fixed value of \( \beta = 2.515 \) as a special case. This is because the W-M model considers the average screening in 2D excitons with binding energies given by \( 4 \times (13.6\mu/\epsilon^2) \) [27]. However, the exciton model given by Jiang et al. [26] results in significant under- or overestimation of binding energies. Moreover, the FCP model is also demonstrated to intercept binding energies for eight bulk materials at \( \beta = 3 \), benchmarked using experimentally reported data [35–46].

The fractional-dimension parameter \( \beta \) is linked to the screening effect due to the fractional Coulomb potential. It is related to the dimensionality in terms of the hydrogenic Bohr radius, explained through the equivalence of the proposed FCP model to an infinite QW model and, in fact, is not directly related to the physical dimensions. It has been shown in Fig. 4 that \( \beta = 3 \) and 2.55 ≤ \( \beta \) ≤ 2.7 represent the bulk and 2D screening, respectively. The Coulomb potential in fractional space provides an additional parameter in the form of \( \beta \), in addition to \( \mu \) and \( \epsilon \), which allows us to incorporate a screening correction in material systems induced due to the varying thickness, substrates, and stress layers and the practical conditions under which the experimental and numerical calculations are performed.

The result in Fig. 5 illustrates an error analysis of the proposed FCP model in comparison with existing models by using BSE-reported data for 58 monolayer materials as a reference. The BSE data are calculated accurately by the FCP model fitted with the respective \( \beta \) values, whereas the W-M data, having an inherently fixed \( \beta = 2.515 \), show an overestimation that increases with the binding energies. However, the exciton model by Jiang et al. [26] has a variable \( \beta \) and is shown to exhibit an increase in underestimation for binding energies greater than 0.5 eV. Moreover, the existing models capture reported values in good agreement limited up to 0.5 eV, as also reported by Olsen et al. [25]. This limitation is caused by the incorrect dielectric screening in the existing models, which is validated by the FCP model, with the identification of actual average screening represented at \( \beta_{\text{mean}} = 2.625 \). This corrected \( \beta \) is found to result in binding energies that fall comparatively, in good agreement with the reported BSE data up to 1.5 eV. The result in Fig. 6 shows an average reduction in the relative MSE for the FCP model with \( \beta_{\text{mean}} = 2.625 \) to less than 12.8%, which is a reduction of approximately one third and one half in comparison to W-M and Jiang et al. [26], respectively.
It is to be noted that the simple screened hydrogen model with the classical Coulomb potential with a $1/r$ dependence demonstrates W-M excitons of a delocalized nature and hence can model binding energies of a few hundreds of millielectronvolts correctly. Since the dielectric screening in some 2D materials can be greatly reduced, the exciton binding energy may reach higher values (up to 1 eV and above). However, their corresponding quasiclassical radius of the ground-state orbital may still remain substantially larger than the lattice constant [49]; such excitons can be regarded as W-M excitons and are sometimes referred to as tightly bound 2D W-M excitons. Here, the materials with higher binding energies are presumed to fall into this category of tightly bound 2D W-M excitons and our FCP model with its $1/r^\beta$-dependence can model them correctly. Once the exciton radius becomes comparable to the lattice constant, the strongly W-M picture becomes inapplicable and a non-Coulombic electron-hole interaction takes place [49,50], which is beyond the scope of the current study. Moreover, binding energies smaller than 0.35 eV are not subject to experiment due to limited availability of the reference data; the materials included in this work have a high dynamic and thermodynamic stability with the available reference values of the BSE binding energy, the $G_0W_0$ band gap, the effective mass, and the 2D polarizability [19].

The FCP model intercepts the BSE-reported 2D binding energies based on a hydrogenic solution with the Coulomb potential represented in the fractional space by including an effective linear screening based on 2D polarizability and additionally allows for the correction in 2D screening through $\beta$, resulting in a Bohr radius corresponding to a 2D regime. Further, an exciton radius of 5.53 Å is calculated for monolayer MoS$_2$ as $R_{\text{exc}} = a_\beta(\epsilon/\mu)$, corresponding to a binding energy of 0.547 eV, intercepted at $\beta = 2.631$. Here, $\mu = 0.236$, $\epsilon = 4.003$, and $a_\beta = 0.326\text{Å}$ is calculated as $w/19.75$, where $w$ is equal to 6.44 Å computed at $\beta = 2.631$, using the result in Fig. 3. The calculated value of 5.53 Å is in good agreement with the theoretically reported value of approximately 5.5 Å [51] corresponding to an experimentally reported monolayer thickness of approximately 0.65 nm [52]. Although an exciton radius of 1 nm has also been reported [21,53], corresponding to varying values of binding energies for free-standing monolayers of 0.96 eV and 0.54 eV, the authors do not explain why the exciton radius does not change: a change in the radius is linked to the screening [54] and the screening effect has been shown to change the binding energies [55]. We believe that such discrepancies can arise due to different approaches chosen to initiate the numerical calculations and that a further investigation in the future will prove to be fruitful.

A smooth transition of $\beta$ with structural confinement from bulk to the monolayer, given the material data for the respective number of layers, is presented in Fig. 7. This demonstration is based on a power-law fit to the reported MoS$_2$ binding energies corresponding to a decreasing number of layers, intercepted with the FCP model through $\beta$ as given in Table I. In practice, the variation of the binding energy is inversely proportional to the dielectric constant, whereas the dielectric constant is known to have a direct relationship with the structural confinement [56,57], due to which the proposed FCP model can provide an approximate estimate of the layer thickness corresponding to the desired binding energy through the mapping of the fractional-dimension parameter $\beta$, as demonstrated in Fig. 8. The result in Fig. 8 is an extension of Fig. 7, which shows a relationship between the fractional-dimension parameter $\beta$ and the number of layers ($L$), given by $\beta(L)$. Here, $\beta(L)$ follows a power-law model of the form

$$
\beta = \frac{a_\beta}{\mu(\epsilon/\mu)}^{\beta(L)}
$$

FIG. 6. The FCP calculation with $\beta_{\text{mean}} = 2.625$ reduces the relative average MSE for 58 monolayer materials up to one half and to one third in comparison to Jiang et al. [26] and W-M, respectively. Moreover, a comparison with Olsen et al. [25] shows an approximate reduction in the error of up to one fourth (for details, see the Supplemental Material [48]).

FIG. 7. A demonstration of the smooth transition of $\beta$ with structural confinement from bulk to the monolayer, given the material data for the respective number of layers, is presented in Fig. 7. This demonstration is based on a power-law fit to the reported MoS$_2$ binding energies corresponding to a decreasing number of layers, intercepted with the FCP model through $\beta$ as given in Table I. In practice, the variation of the binding energy is inversely proportional to the dielectric constant, whereas the dielectric constant is known to have a direct relationship with the structural confinement [56,57], due to which the proposed FCP model can provide an approximate estimate of the layer thickness corresponding to the desired binding energy through the mapping of the fractional-dimension parameter $\beta$, as demonstrated in Fig. 8. The result in Fig. 8 is an extension of Fig. 7, which shows a relationship between the fractional-dimension parameter $\beta$ and the number of layers ($L$), given by $\beta(L)$. Here, $\beta(L)$ follows a power-law model of the form

$$
\beta = \frac{a_\beta}{\mu(\epsilon/\mu)}^{\beta(L)}
$$

FIG. 7. A demonstration of the smooth transition of $\beta$ with respect to the binding energy for MoS$_2$, given $\mu$ and $\epsilon$ data for the respective numbers of layers. The blue dotted line represents a power-law fit to the data points given in Table I.
TABLE I. The calculation details for FCP-model-based interception of the reported MoS$_2$ binding energies corresponding to a structural confinement from bulk to the monolayer.

| Structure     | $\mu$ [35] | $\epsilon$ [35] | Binding energy (eV) [35] | Number of layers ($L$) [59] | $\beta_{\text{FCP}}^a$ |
|---------------|------------|-----------------|--------------------------|----------------------------|------------------------|
| Bulk          | 0.4        | 10.71           | 0.04                     | 31$^b$                     | 3                      |
| Six-layer     | 0.3        | 7.92            | 0.08                     | 6 [59]                     | 2.913                  |
| Four-layer    | 0.25       | 7.16            | 0.09                     | 4 [59]                     | 2.875                  |
| Bi-Layer      | 0.25       | 5.51            | 0.424                    | 2 [59]                     | 2.531                  |
| Monolayer     | 0.19       | 3.43            | 0.897                    | 1 [47]                     | 2.506                  |

$^a$The FCP-model interception of binding energies for the respective layers through tuning of $\beta$.

$^b$Bulk thickness (approximately 20 nm)/monolayer thickness (0.65 nm) [52].

\[(c_1L^2 + c_3)\]

and indicates a sharp decrease in the screening for the 2D regime (very small $L$) compared to the bulk regime (large $L$), attributed to the strong excitonic effects due to structural confinement. This allows an approximate calculation of the binding energies for a changing number of layers as $E_{\beta,L} = E_0(\alpha \beta(L)^b + c)(\mu/\epsilon^2)$, where $a$, $b$, and $c$ remain the same as in Eq. (5), highlighting the usefulness of the FCP model in practical design problems. It is worthwhile to mention that an earlier model reported by Thilagam has reported the kinetic energy part of the two-particle fractional-dimension Schrödinger equation with a classical Coulomb potential [58]. On the contrary, our FCP model demonstrates that the fractional Coulomb potential corresponds to structural changes from bulk to the 2D regime and thus provides a better representation of dielectric screening in confined materials.

As an example for many applications, recent studies on a number of photovoltaic systems based on 2D materials [60–63] have been demonstrated to highlight the influence of various dielectric environments and structural configurations on the critical role of the binding energy in solar applications for a favorable dissociation of photogenerated excitons into free carriers at room temperature. Further, the 2D binding energy is reported to make a significant contribution to band-gap renormalization and is shown to vary due to the screening induced by the external dielectric environment, leading to shifts in the optical spectrum [64–66]. Thus 2D-material-based optical detection, which requires a strict optical frequency and a narrow line width, would demand an accurate determination of the binding energy. Here, the FCP model will prove to be a promising tool due to its ability to produce accurate binding energies for a wide range of 2D materials with the average screening felt by 2D excitons corrected to represent a more realistic dielectric environment, hence contributing toward the accurate determination of optoelectronic properties. Additionally, it has the potential to track the variation in binding energy due to a change in material thickness from a monolayer to many layers and thus can allow for binding-energy tunability to achieve efficient photovoltaic conversion as reported in the literature [67,68].

Furthermore, strain in 2D materials is shown to induce band-gap shifts with excitonic effects [5,69,70] and various experimental and numerical studies [71–73] have been reported recently to account for strained excitonic effects. In future, our proposed FCP model can be extended to calculate the strained binding energies by establishing a physical relationship between $\beta$ and the lattice parameters corresponding to the strain levels. Such an extension can potentially be used as a tool to control the optical properties of strained 2D materials [17].

IV. CONCLUSION

In conclusion, the proposed model gives a generalized analytical expression to calculate the binding energies for a wide range of materials ranging from bulk to the 2D regime using the reported material parameters $\mu$ and $\epsilon$. The fractional-dimension parameter $\beta = 3$ and $2.55 \leq \beta \leq 2.7$ corresponds to the actual dielectric screening in bulk and 2D materials, respectively, and thus results in an accurate calculation of the binding energies for 58 monolayer and eight bulk materials benchmarked using reported data. An

\[3.385, 1.707\]

FIG. 8. A demonstration of the smooth transition of $\beta$ with respect to the number of layers in MoS$_2$, showing the usefulness of the FCP model in the design process for practical applications. The blue dotted line shows that $\beta(L)$ follows a power-law model as $(c_1L^2 + c_3)$, which is obtained by performing a fit to the data points given in Table I, where $c_1 = -0.5233$, $c_2 = -0.8394$, and $c_3 = 3.029$ with confidence bounds of $(-1.19, 0.1439)$, $(-3.385, 1.707)$, and $(2.413, 3.646)$, respectively. The black markers indicate the FCP data.
average screening in 2D excitons represented by $β_{\text{mean}} = 2.625$ comparatively reduces the relative MSE, on average, by up to one third with most of the materials captured by our model up to 1.5 eV, in contrast to 0.5 eV in existing models. Finally, for a given material, we show that there exists a scaling law between $β$ and structural confinement from bulk to the monolayer, which assists in the tuning of the binding energy by varying the material thickness. The proposed FCP model will prove useful in the design and engineering of optoelectronic devices based on 2D heterostructures, due to the critical role of the binding energy in the efficient photoconversion operation. The FCP model can provide a useful tool with its analytical approach through providing accurate binding-energy estimates for 2D materials under the impact of practical dielectric environments, thus contributing toward the optimal design of optoelectronic devices.

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APPENDIX: DETAILED DERIVATION AND FULL SOLUTION OF SCREENED HYDROGEN MODEL WITH FRACTIONAL COULOMB POTENTIAL (FCP)

The FCP model is developed based on an arbitrary potential embedded in the infinite quantum well, as illustrated in Fig. 9, following the eigenvalue calculation method reported in Ref. [74].

The radial part of the simple hydrogen model in spherical coordinates incorporating the fractional Coulomb potential represents the FCP model as follows:

$$
\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_{\text{frac}}(r)\right] \psi(r) = E \psi(r), \quad (A1)
$$

where $μ = 0.9995m_0$ is the exciton reduced mass, $V_{\text{frac}}(r) = k_βe^2/r^{β-2}$ is the fractional Coulomb potential, $r$ is the radial distance equivalent to the infinite QW width, and $β$ is the fractional-dimension parameter linked to the screened Coulomb potential.

The formulation of the eigenvalue problem for a fractional Coulomb potential embedded in an infinite QW is given by $\sum_{n=1}^{n_{\text{max}}} H_{nm}c_n = Ec_n$, and the Hamiltonian-matrix elements are given by

$$
H_{nm} = \left[\langle \phi_n | H_0 + V_{\text{frac}}| \phi_n \rangle \right] = \delta_{nm}E_n + V_{\text{frac}}(r), \quad (A2)
$$

where $H_0|\phi_n⟩ = E_n|\phi_n⟩$ represents the infinite QW. The eigenstates of the infinite QW, $\phi_n(r) = \sqrt{2/n}\sin(nπr/a)$, with eigenvalues $E_n = n^2\hbar^2a^2/2m_0a^2$, allow for the Fourier-series expansion of the embedded wave function as $|ψ⟩ = \sum_{n=1}^{n_{\text{max}}} c_n|\phi_n⟩$, where $\int_0^∞ |ψ(r)|^2 dr = 1$. The infinite QW enforces the embedding wave function $ψ(r)$ to satisfy the von Kármán boundary conditions as $ψ(0) = 0$ and $ψ(r = a) = 0$. Here, $m_0 = 9.11 \times 10^{-31}$ kg and $a = 20a_0$ is the width of the infinite quantum well. The fractional Coulomb potential over the radial distance is expressed as

$$
V_{\text{frac}}(r) = -\frac{2k_βe^2}{a} \int_0^a \sin \left(\frac{nπr}{a}\right) \frac{1}{r^{β-2}} \sin \left(\frac{mπr}{a}\right) dr, \quad (A3)
$$

where $k_β = Γ(β/2)/(2π^{β/2}(β - 2)ε_0)$. After trigonometric transformations, we arrive at

$$
V_{\text{frac}}(r) = -\frac{k_βe^2}{a} \left[ G(n + m) - G(n - m) \right], \quad (A4)
$$

where

$$
G(n + m) = \int_0^a \left[ 1 - \cos \left(\frac{πr}{a} \right) \right] dr, \quad (A5)
$$

$$
G(n - m) = \int_0^a \left[ 1 - \cos \left(\frac{πr}{a} \right) \right] dr.
$$
FIG. 11. The FCP-model convergence calculated by varying $n_{\text{max}}$ for $a/a_0 = 20$.

The plots in Figs. 10 and 11 show the convergence of the FCP model for the ground-state energy for $2 < \beta \leq 3$ with respect to $a/a_0$ and $n_{\text{max}}$, respectively, where $n_{\text{max}}$ represents the Hamiltonian matrix size, which is dependent on the cutoff energy of the wave function, and $a/a_0$ represents the radial distance equivalent to an infinite QW width, which is important for convergence. We perform our calculation for $n_{\text{max}} = 400$ and $a/a_0 = 50$.

The dimensionless version of the Hamiltonian matrix equation for the FCP model is represented as

$$\sum_{m=1}^{n_{\text{max}}} h_{nm} c_m = e c_n, \quad (A6)$$

where $h_{nm} = E_{nm}/E_0$, $e = E/E_0$, and $E_0 = \hbar^2/2m_0a_0^2 \approx 13.606$ eV, resulting in the following expression for the numerical calculation of the eigenvalues:

$$h_{nm} = \delta \left( \frac{\pi n a_0}{a} \right)^2 - \frac{4\pi \left(1-\frac{\pi}{\beta} \right) \Gamma(\beta/2) a_0}{(\beta - 2)} \left[ G(n + m) - G(n - m) \right]. \quad (A7)$$

The integrals are computed using trapezoidal integration and the dimensionless Hamiltonian matrix for the FCP model is solved for the first bound states by employing block diagonalization using the Jacobian rule.

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