TWO-DIMENSIONAL WANNIER – MOTT EXCITON IN A UNIFORM ELECTRIC FIELD

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A new treatment of the problem of a two-dimensional Wannier – Mott exciton in a uniform electric field, based on the parabolic coordinates, is presented. The quasi-stationary Hamiltonian is regularized and efficient numerical methods are applied. The dependence of the exciton binding energy on electric field is computed. The results are very close to ones obtained with the perturbation calculus.

Introduction

Three-dimensional Wannier – Mott exciton (WME) is usually described within the effective-mass approximation [1 – 11]. The essential effect of an external uniform electric field **E** is that the problem becomes nonstationary. An exciton can be ionized and its lifetime is finite, which involves the use of the time-dependent Schrödinger equation (SE). However, assuming that the exciton lifetime is sufficiently long, one can treat the problem as a quasi-stationary one and employ the stationary SE:

$$\left[-\frac{\hbar^2}{2m_e^*}\nabla^2_{\mathbf{r}_e} - \frac{\hbar^2}{2m_h^*}\nabla^2_{\mathbf{r}_h} - \frac{e^2}{\varepsilon|\mathbf{r}_e - \mathbf{r}_h|} + e\,\mathbf{E}\cdot(\mathbf{r}_e - \mathbf{r}_h)\right]\Phi(\mathbf{r}_e, \mathbf{r}_h) = (\varepsilon_{\text{exc}} - \varepsilon_g)\Phi(\mathbf{r}_e, \mathbf{r}_h), \quad (1)$$

where ε_g is the energy gap and ε_{exc} is the total exciton energy. It is analogous to the hydrogen atom problem [12].

Equation (1) is not solvable analytically for $E \neq 0$. In the parabolic coordinates, the 3*D* WME problem transforms to two coupled one-dimensional eigenproblems [3, 5 – 8, 12]. The case where the motion of an electron and a hole is restricted to two dimensions (it can be modelled by a very deep and narrow quantum well and is analogous to a two-dimensional atom) can be treated similarly [9]. The 2*D* problem was solved analytically in [13] for $E = 0$. The case of $E \neq 0$ was investigated numerically in [9]. Both 3*D* and 2*D* cases with $E = 0$ were also considered in the momentum space [11].

Here, we present a new approach to the 2*D* WME problem. It is based on a parabolic coordinate system defined in a different way than in [9]. This approach

1) is a generalization of the standard method presented in [12] for a 3*D* hydrogen atom;

2) results in the Hamiltonian regularization;

3) allows us to perform a numerical analysis of the problem with the help of efficient modern methods of a computer linear algebra.

In the standard variable separation procedure, one introduces the center-of-mass coordinate **R**, relative one **r**, and reduced mass μ. It allows us to write a total envelope function in the form $\Phi(\mathbf{R}, \mathbf{r}) = \exp(i\mathbf{K}\cdot\mathbf{R})\psi(\mathbf{r})$ that gives $\varepsilon_{\text{exc}} = \frac{\hbar^2 K^2}{2(m_e^* + m_h^*)} + \varepsilon + \varepsilon_g$. The wave function ψ satisfies the dimensionless SE

$$\left[-\nabla^2 - \frac{2}{r} + 2\mathbf{E}\cdot\mathbf{r}\right]\psi(\mathbf{r}) = \varepsilon\psi(\mathbf{r}). \quad (2)$$

Eq.(2) is written in the atomic units of length $a_0 = \varepsilon\hbar^2/(\mu e^2)$ (effective Bohr radius), energy $W_0 = \mu e^4/(2\varepsilon^2\hbar^2)$ (effective Rydberg), and field $E_0 = \frac{e}{\varepsilon a_0^2}$.

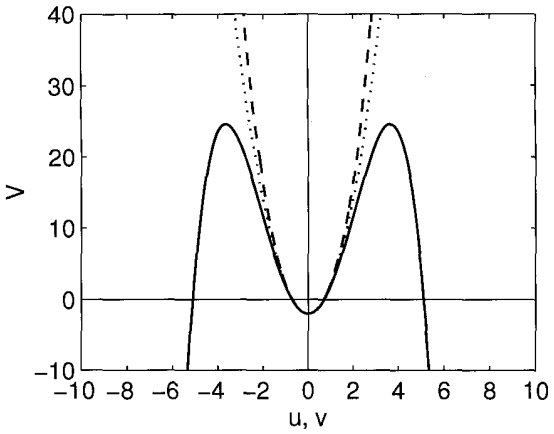

Fig.1. Quasipotentials: ν_+ (dashed line), ν_- (solid) for $E = 0.15$ and for $E = 0$ (dotted)

1. Two-Dimensional Exciton for $E = 0$ in Polar Coordinates

In the polar (or cylindrical) coordinate system (r, φ), Eq.(2) reads for $E = 0$ as

$$\left[-\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2} - \frac{2}{r}\right]\psi(r, \varphi) = \varepsilon\psi(r, \varphi).$$

It is solvable analytically [13]. The normalized eigenfunctions of bound states are

$$\psi^c_{n, m}(r, \varphi) = \frac{\lambda_n^{3/2}}{\sqrt{\pi}}\sqrt{\frac{(n - |m|)!}{(n + |m|)!}} \times$$

$$\times\, e^{-\lambda_n r}[2\lambda_n r]^{|m|} L^{2|m|}_{n-|m|}(2\lambda_n r) e^{im\varphi} \qquad (3)$$

for $|m| \le n = 0, 1, 2, \ldots$, and $\lambda_n = \left(n + \frac{1}{2}\right)^{-1}$; '$c$' stands for 'cylindrical'. Their eigenenergies are $\varepsilon_{n, m} = \varepsilon_n = -\left(n + \frac{1}{2}\right)^{-2}$. The symbol $L^a_N(x)$ denotes generalized Laguerre polynomials [18].

2. Two-Dimensional Exciton in Parabolic Coordinates

This section shows the idea of our new approach to the problem. Let us write the Schrödinger equation (2) in the parabolic coordinate system by using formulae (10) and (12):

$$\left[-\frac{1}{u^2 + \upsilon^2}\left(\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial \upsilon^2}\right) - \frac{4}{u^2 + \upsilon^2} + \right.$$

$$\left. + (u^2 - \upsilon^2)E\right]\psi(u, \upsilon) = \varepsilon\psi(u, \upsilon). \qquad (4)$$

We factorize $\psi(u, \upsilon) = f(u)g(\upsilon)$ and remove the singularity multiplying (4) by $(u^2 + \upsilon^2)$. After separating the variables, we get two coupled equations with separation parameter C:

$$\begin{cases} \left[-\dfrac{d^2}{du^2} - \varepsilon u^2 + Eu^4 - 2\right]f(u) = \\ = \left[-\dfrac{d^2}{du^2} + \nu_+(u)\right]f(u) = -Cf(u), \\ \left[-\dfrac{d^2}{d\upsilon^2} - \varepsilon\upsilon^2 - E\upsilon^4 - 2\right]g(\upsilon) = \\ = \left[-\dfrac{d^2}{d\upsilon^2} + \nu_-(\upsilon)\right]g(\upsilon) = Cg(\upsilon). \end{cases} \qquad (5)$$

Eqs.(5) are one-dimensional Schrödinger-like equations. They are eigenproblems for the separation parameter C. The binding energy ε is a parameter of the functions $\nu_\pm$, which we will call quasipotentials (they correspond to potentials in an ordinary SE):

$$\nu_\pm(\varepsilon; w) = -\varepsilon w^2 \pm Ew^4 - 2, \qquad (6)$$

where w denotes the coordinate u or υ. They are shown in Fig.1.

The numerical procedure of solving Eq.(5) should then consist in finding such a value of $\varepsilon(E)$ for which the eigenvalues C and $-C$ match both Eqs.(5).

Here, we note that the alternative definition of the parabolic coordinates (13) applied in [9] also leads to variable separation. One gets then a set of two ordinary SE (with ε being the eigenvalue), but the singularity is not removed and the numerical problem is more difficult.

The value of $f(0)$ is unknown. We cannot impose the convenient boundary condition $f(u = 0) = 0$ because it would imply $\psi(0, 0) = 0$. In order to avoid this difficulty, let us extend the domain of u to negative values (we make use of the properties of the conformal mapping (11)). That involves the condition

$$\psi(u, \upsilon) = \psi(-u, -\upsilon) \qquad (7)$$

(see Appendix). Quasipotentials (6) are even functions. Therefore, from (7), $f(u)$ and $g(\upsilon)$ have to be either both even or both odd.

3. Analytic Results for $E = 0$

The case of $E = 0$ is solvable analytically. Eqs.(5) read then as (the double sings correspond to the first orsecond equation, respectively)

$$\left[-\frac{d^2}{dw^2} + \lambda^2 w^2\right] f_\pm(w) = (2 \pm C) f_\pm(w), \qquad (8)$$

where w means u or υ, f_- and f_+ denote f and g, and $\lambda^2 = -\varepsilon$. We note that (8) is an 'inverted" quantum linear oscillator eigenproblem with the eigenvalues $2 \pm C = (2n_\pm + 1)\lambda$ for $n_\pm = 0, 1, 2, \ldots$, and the eigenfunctions $f_{n_\pm}(x) = \exp\left(-\frac{1}{2}\lambda x^2\right) \times$ $\times H_{n_\pm}(\sqrt{\lambda}x)$, where $H_N(x)$ denotes Hermite polynomials [18].

It is easy to show that $\lambda_{n_+, n_-} = 2/(n_+ + n_- + 1)$, where n_+ and n_- denote parabolic quantum numbers. From (7), we get $n_+ + n_- = 2n$, where $n = 0, 1, 2, \ldots$ denotes the principal quantum number describing the energy of an eigenstate $\varepsilon_{n_+, n_-} = \varepsilon_n = -\lambda_n^2 = -\left(n + \frac{1}{2}\right)^{-2}$. Normalized wave functions have the form

$$\psi_{n_+, n_-}(u, \upsilon) = I_{n_+, n_-} \times$$

$$\times \exp\left[-\frac{1}{2}\lambda_n(u^2 + \upsilon^2)\right] H_{n_-}(\sqrt{\lambda_n}u) H_{n_+}(\sqrt{\lambda_n}\upsilon),$$

where I_{n_+, n_-} is the normalization factor which depends only on n: $I_{n_+, n_-} = I_n$. We can change the indices of ψ in order to put n among them. As the secondary quantum number, we choose $j = \frac{1}{2}(n_+ - n_-) = -n, -n+1, \ldots, n-1, n$.

Finally, the normalized eigenfunctions of bound states in the parabolic coordinates are

$$\psi^p_{n, j}(u, \upsilon) = \frac{\lambda_n^{3/2}}{\sqrt{\pi}} \frac{i^{n+j} \exp\left[-\frac{1}{2}\lambda_n(u^2 + \upsilon^2)\right]}{2^n \sqrt{(n-j)!(n+j)!}} \times$$

$$\times H_{n-j}(\sqrt{\lambda_n}\, u) H_{n+j}(\sqrt{\lambda_n}\, \upsilon), \qquad (9)$$

where p stands for 'parabolic'. The arbitrary factor i^{n+j} results in a simplification of the transformation matrices discussed elsewhere.

4. Numerical Results

A solution of (5) is equivalent to finding a zero of the fuction

$$h(E; \varepsilon) = C_0^+(E, \varepsilon) + C_0^-(E, \varepsilon)$$

for a given E. Here, $C_0^\pm$ denotes the lowest eigenvalues of the separation constant C obtained from the first and the second equation in (5), for the respective signs.

We computer the eigenvalues $C_0^\pm$ with the help of precise and efficient grid matrix methods [14 – 16]. The applied methods solve the Schrödinger equation within a finite interval with the boundary conditions (BC) assuming that the wave function vanishes at its ends. It is equivalent to putting infinite potential barriers there. These BC cause no essential error for the quasipotential $v_+(u)$ if the considered interval is sufficiently wide. For the quasipotential $v_-(\upsilon)$, the function $g(\upsilon)$ does not vanish for $|\upsilon| \to \infty$, and the error caused by BC has to be minimized. We did so by using the modified potential shown in Fig.2. The interval d has been enlarged until it did not change the results any more.

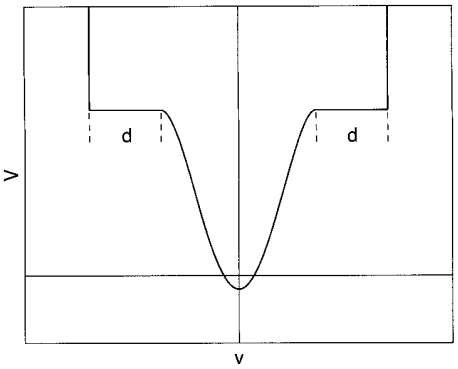

Fig.2. Modified quasipotential $v_-(\upsilon)$

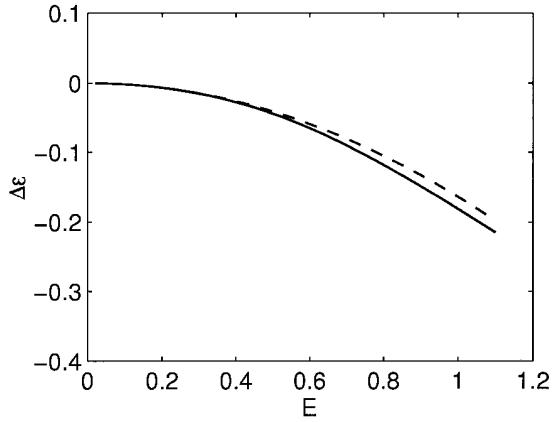

Fig.3. Numerical results: $\Delta\varepsilon_0^{\text{comp}}$ (solid line) and $\Delta\varepsilon_0^{\text{pert}}$ (dashed)

The computational results are presented in Fig.3. We compare the computed correction to the ground state energy $\Delta\varepsilon_0^{\text{comp}}(E)$ with one obtained from the second-order perturbation calculus [9]:

$$\Delta\varepsilon_0^{\text{pert}}(E) = -\frac{21}{128}E^2 \approx -0.164E^2.$$

The results obtained with these two methods do not differ much ($|\Delta\varepsilon_0^{\text{comp}}(E)|$ is higher than $|\Delta\varepsilon_0^{\text{pert}}(E)|$

by less than 1% for $E < 0.05$ and about 10% for $E \sim 1$). Therefore, a two-dimensional exciton, as a relatively strongly bound system, is weakly polarizable and the perturbation calculus gives surprisingly good results. This observation is in agreement with one made in [9]. This result is different than that in the 3*D* case [9, 10].

We also computed the tunneling coefficient T within the WKB-like 1*D* approximation (tunneling along the x direction). It reaches a relatively high value ($T \sim 0.1$) at $E \sim 0.7$.

Conclusions

The main results presented here are as follows:

1. The Schrödinger equation describing a two-dimensional Wannier – Mott exciton in a uniform electric field can be transformed to two coupled one-dimensional eigenproblems of the type of anharmonic linear oscillator.
2. The applied coordinate transformation results in the Hamiltonian regularization, which allows us to use simple and efficient numerical algorithms.
3. The problem is nonstationary and the applied quasistationary approach has an approximate character for strong external fields.
4. The numerical calculations shown that the exciton ground state disappears at $E \approx 1.1$ (in atomic units).
5. The computed ground state energy correction does not differ much from the results of the perturbation calculus. It means that a 2*D* exciton is less polarizable than a 3*D* one.

In a further investigation, it would be important to solve a time-dependent Schrödinger equation (at least approximately, using the complex energy: formalism $\tilde{\varepsilon} = \varepsilon - i\Gamma$) and to evaluate the exciton lifetime. It also seems interesting to investigate a 2*D* exciton with the 2*D* Coulomb potential ($\ln r$).

APPENDIX. Parabolic Coordinate System

The parabolic coordinates (u, υ) are defined on the x-y plane as [17]

$$x = \frac{1}{2}(u^2 - \upsilon^2), \quad y = u\upsilon. \tag{10}$$

We choose $u \geq 0$ and $\mathrm{sgn}\upsilon = \mathrm{sgn}y$. Relations (10) can be written as a two-branch conformal mapping

$$x + iy = re^{i\varphi} = (u + i\upsilon)^2; \tag{11}$$

the connection with the polar coordinates (r, φ) is also simple. The plane (x, y) is mapped into two equivalent half-planes $u \geq 0$ and $u \leq 0$. Therefore, it is possible to consider only symmetric functions $f(-u, -\upsilon) = f(u, \upsilon)$, however on the whole plane (u, υ).

In the parabolic coordinates (10), we have

$$\nabla^2 = \frac{1}{u^2 + \upsilon^2}\left(\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial \upsilon^2}\right), \quad dS = (u^2 + \upsilon^2)du d\upsilon. \tag{12}$$

The parabolic coordinates are sometimes defined in a different way [9]:

$$x = \frac{1}{2}(u - \upsilon), \quad y = \sqrt{u\upsilon}; \tag{13}$$

these relations cannot be written as a conformal mapping.

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