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 fielfd, based on the parabolic coordinates, is presented. The quasi-stationary Hamiltonian is regularized, and the efficient numerical methods are applied. The dependence of the exciton binding energy on the electric field is computed. The results are very close to those obtained by the perturbation theory calculations.

The 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 $\mathbf{E}$ is that the problem becomes non-stationary. The 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

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

where ε_g is the energy gap and $\varepsilon_{\rm exc}$ 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 $3D$ WME problem transforms to two coupled one-dimensional eigenproblems [3,5–8,12]. The case when both the electron and the hole motion is restricted to two dimensions (which 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 $2D$ problem was solved analytically in [13] for $E=0$. The case of $E\neq 0$ was investigated numerically in [9]. Both $3D$ and $2D$ cases with $E=0$ were also considered in momentum space [11].

In this paper we present a new approach to the $2D$ 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 the $3D$ hydrogen atom; 2) results in the Hamiltonian regularization; 3) allowed us to perform a numerical analysis of the problem with the help of the efficient modern methods of linear algebra.

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

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

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

1. Two-dimensional exciton for $E=0$ in polar coordinates

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

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

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

$$\psi^c_{n,m}(r,\varphi)=\frac{\lambda_n^{3/2}}{\sqrt{\pi}}\sqrt{\frac{(n-|m|)!}{(n+|m|)!}}\times e^{-\lambda_n r}[2\lambda_n r]^{|m|}L^{2|m|}_{n-|m|}(2\lambda_n r)e^{im\varphi}\qquad(3)$$

for $|m|\leq n=0,1,2,\ldots$, and $\lambda_n=(n+1/2)^{-1}$; c stands for 'cylindrical'. The eigenenergies are $\varepsilon_{n,m}=\varepsilon_n=-(n+1/2)^{-2}$. The symbol $L^a_N(x)$ denotes the generalized Laguerre polynomials [14].

2. Two-dimensional exciton in parabolic coordinates

This section shows the idea of out new approach to the problem. Let us write the SE (2) in the parabolic coordinate system using formulae (10) and (12)

$$\left[-\frac{1}{u^2+v^2}\left(\frac{\partial^2}{\partial u^2}+\frac{\partial^2}{\partial v^2}\right)-\frac{4}{u^2+v^2}+(u^2-v^2)E\right]\psi(u,v)=\varepsilon\psi(u,v).\qquad(4)$$

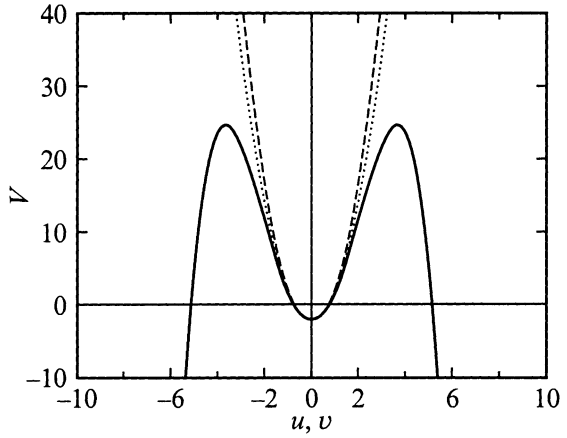

Figure 1. The quasipotentials: V_+ (dashed line), V_- (solid line) for $E = 0.15$ and for $E = 0$ (dotted line).

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

$$\left[-\frac{d^2}{du^2} - \varepsilon u^2 + Eu^4 - 2\right] f(u) = \left[-\frac{d^2}{du^2} + V_+(u)\right] f(u) = -Cf(u),$$

$$\left[-\frac{d^2}{dv^2} - \varepsilon v^2 - Ev^4 - 2\right] g(v) = \left[-\frac{d^2}{dv^2} + V_-(v)\right] g(v) = Cg(v). \quad (5)$$

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

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

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

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

Here we must note that the alternative definition of 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). That involves the condition

$$\psi(u, v) = \psi(-u, -v) \quad (7)$$

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

3. Analytical results for $E = 0$

The case of $E = 0$ is solvable analytically. Equations (5) then read (the double signs correspond to the first and the second equation, respectively)

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

where w means u or v, f_- and f_+ denote f and g, and $\lambda^2 = -\varepsilon$. We can 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 $f_{n_\pm}(x) = \exp(-(1/2)\lambda x^2) H_{n_\pm}(\sqrt{\lambda}\, x)$, where $H_N(x)$ denotes Hermite polynomials [14].

It is easy to show that $\lambda_{n_+,n_-} = 2/(n_+ + n_- + 1)$, where n_+ and n_- denote the 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 $\varepsilon_{n_+,n_-} = \varepsilon_n = -\lambda_n^2 = -(n + 1/2)^{-2}$. Normalized wave functions have the form

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

where I_{n_+,n_-} is the normalization factor depending 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 $j = 1/2(n_+ - n_-) = -n, -n + 1, \ldots, n - 1, n$.

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

$$\psi^p_{n,j}(u, v) = \frac{\lambda_n^{3/2}}{\sqrt{\pi}} \frac{i^{n+j} \exp\left[-(1/2)\lambda_n(u^2 + v^2)\right]}{2^n \sqrt{(n - j)!(n + j)!}} \times H_{n-j}(\sqrt{\lambda_n}\, u) H_{n+j}(\sqrt{\lambda_n}\, v), \quad (9)$$

where 'p' stands for 'parabolic'.

4. Numerical results

Solution of (5) is equivalent to finding a zero of the function

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

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

We computed the eigenvalues $C_0^\pm$ with the help of precise and efficient grid matrix method [15–17].

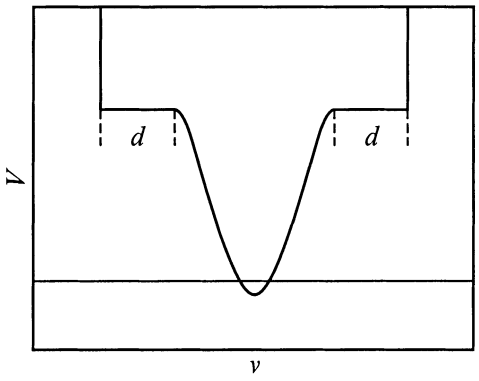

Figure 2. The modified quasipotential $V'_{-}(v)$.

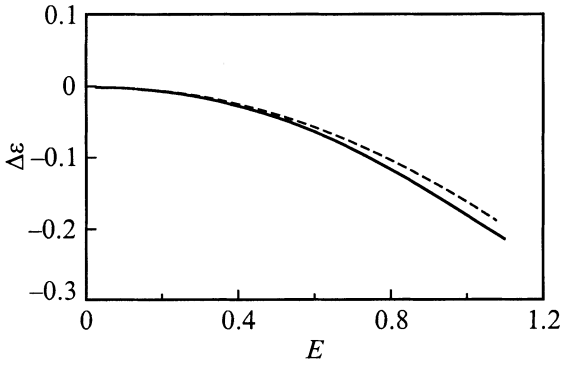

Figure 3. Numerical results: $\Delta\varepsilon_0^{\text{comp}}$ (solid line) and $\Delta\varepsilon_0^{\text{pert}}$ (dashed line).

The applied methods solve the SE within a finite interval with the boundary conditions assuming the wave function to vanish at its ends. It is equivalent to putting infinite potential barriers there. These boundary conditions cause no essential error for the quasipotential $V_{+}(u)$, if the considered interval is sufficiently wide. For the quasipotential $V_{-}(v)$ the function $g(v)$ does not vanish for $|v| \to \infty$ and the error caused by boundary conditions 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.

The results of computation 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 the 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]. The results is different for the $3D$ case [9,10].

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

The main results presented in this paper 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 anharmonic linear oscillator-type.

2) The applied coordinate transformation results in Hamiltonian regularization, which allows us to use simple and efficient numerical algorithms.

3) The problem is non-stationary and the applied quasi-stationary approach has an approximate character for strong external fields.

4) The numerical calculations show that the exciton ground state disappears at $E \simeq 1.1$ (in atomic units).

5) The computed ground state energy correction does not differ much from the results of the perturbation calculus. It means that the $2D$ exciton is less polarizable than the $3D$ one.

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

Appendix: The parabolic coordinate systems

The parabolic coordinates (u, v) are defined on the $x - y$ plane as [18]

$$x = \frac{1}{2}(u^2 - v^2), \qquad y = uv. \tag{10}$$

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

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

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 $f(-u, -v) = f(u, v)$, however on the whole plane (u, v).

In the parabolic coordinates (10) we have

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

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

$$x = \frac{1}{2}(u - v), \qquad y = \sqrt{uv}; \tag{13}$$

these relations cannot be written as a conformal mapping.

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